PART 2

2002 LAKE MICHIGAN MASS BALANCE PROJECT: MODELING TOTAL POLYCHLORINATED BIPHENYLS USING THE MICHTOX MODEL

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2.1 Executive Summary

The MICHTOX model was used to perform a preliminary mass balance modeling assessment for polychlorinated biphenyls (PCBs) in Lake Michigan. Comparison of model predictions to data generated by the Lake Michigan Mass Balance Project (LMMBP) provided a unique opportunity to confirm the MICHTOX model using data not available at the time of its development. Principal results of the MICHTOX assessment include:

1. Total PCBs forcing function estimates from the LMMBP are compatible with the original MICHTOX model estimates for atmospheric deposition and tributary loading. However, atmospheric total PCBs vapor concentrations from the LMMBP are significantly higher than estimated in the original model. Consequently, all total PCBs forcing functions were recalculated, using the LMMBP estimates.

2. Changes to the model formulation and parameterization, recommended by the LMMBP Atmospheric Workgroup, enhance the volatility of total PCBs and increase the volatilization mass transfer rates. As a result of these changes, PCBs equilibrium was shifted significantly towards the atmospheric vapor phase, and this shift occurred more rapidly than previously predicted. The enhanced volatility of total PCBs was found to completely offset the greater absorption resulting from higher vapor concentrations. Mass balance diagnostics also demonstrate that air-water fluxes now clearly predominate the transport pathways for PCBs in Lake Michigan.

3. Model simulations were conducted using different assumptions regarding long-term total PCBs forcing functions. The most reasonable predictions were obtained by assuming that total PCBs forcing functions peaked in 1961-1963. The simulation made using this assumption offered a better prediction of the total PCBs concentrations observed in water, sediment, and fish than the original MICHTOX model simulation.

4. The model was applied to forecast total PCBs concentrations in lake trout for a number of scenarios in which the future PCBs forcing functions were changed from their 1994-1995 estimated values. These changes were intended to represent alternative strategies for managing PCBs in Lake Michigan, and the model was used to forecast the effectiveness of these alternatives in terms of reducing lake trout total PCBs concentrations. The results of the toxic chemical management forecasts demonstrated that properly evaluating the effectiveness of control action depends upon understanding which forcing functions are controllable and what the future trend in forcing functions (especially atmospheric

vapor concentrations) will be in the absence of control actions.

5. The uncertainty of MICHTOX predictions arising from errors in model parameterization and forcing functions was evaluated using Bayesian Monte Carlo (BMC) analyses. Based on the uncertainty in model predictions arising from these factors, observed average total PCBs concentrations should be well within a factor of two of predicted values.

6. The MICHTOX model does not predict equilibrium between air and water total PCBs concentrations.

7. Total PCBs bioaccumulation predictions were not sensitive to initial concentration conditions in fish, after an initial simulation period. Fish total PCBs concentration predictions were demonstrated to be quite sensitive to bioaccumulation model parameterization.

8. Bioaccumulation factors were predicted to vary continuously throughout the model simulations.

9. The MICHTOX model was found to provide a reasonably accurate simulation of total PCBs in the Lake Michigan ecosystem. However, the preliminary MICHTOX assessment will be superceded in the next several years by mass balance models with significantly better resolution and better process and state variable representations. Furthermore, these newer models will be capable of making full use of the LMMBP data; for example, they can be used to model PCBs as individual congeners.

2.2 Recommendations

After revising and successfully running MICHTOX as a screening-level model, a number of issues became apparent which require further consideration. These are as follows:

1. For the forcing function assumption used, the model does not predict equilibrium between the air and water total PCBs concentrations. Other forcing functions scenarios should be done to determine whether this is a general result or a result specific to the chosen function.

2. Chemical assimilation efficiency, diet composition, growth rates, lipid contents, chemical excretion rates, and phytoplankton bioconcentration should be examined in any recalibration of the model.

3. Bioaccumulation factors should be used with caution in Lake Michigan because they are expected to vary with time.

2.3 Introduction

The LMMBP is a coordinated effort among federal, state, and academic scientists to monitor tributary and atmospheric pollutant loads, develop source inventories of toxic substances, and evaluate the fate and effects of these pollutants in Lake Michigan. A key objective of the LMMBP is to construct mass budgets and mass balance models for a limited group of contaminants that are present in Lake Michigan at concentrations that pose a risk to aquatic and terrestrial organisms within the ecosystem. The mass balance modeling is being conducted to support both regulatory and research agendas, as described in the LMMBP Study Plan (U.S. Environmental Protection Agency, 1997). Elements of the LMMBP which provide information for the modeling objective include:

1. Monitoring of atmospheric and tributary toxic chemical sources and estimation of loadings and other forcing functions at spatial and temporal scales necessary for mass balance modeling.

2. Measurement of toxic chemical concentrations in lake water at 41 stations and six cruises (i.e, sampling events) over the course of the two-year mass balance study period.

3. Concurrent measurement of suspended solids, organic carbon, and nutrients in all water column samples.

4. Measurement of toxic chemical and associated state variables in surficial sediments throughout Lake Michigan.

5. Measurement of toxic chemicals in representative biota for pelagic and benthic food chains for two top predator fishes, lake trout and coho salmon, for multiple locations and seasons.

The sampling design and analytical parameters of the LMMBP were specified to support the development of hydrodynamic, sediment transport, eutrophication, contaminant transport/fate, and food web bioaccumulation models (U.S. Environmental Protection Agency, 1997). The various models and submodels that comprise this system are under development by the United States Environmental Protection Agency (USEPA) at the Large Lakes Research Station (LLRS), Grosse Ile, Michigan.

This report presents a preliminary mass balance modeling assessment for PCBs in Lake Michigan using the MICHTOX model (described in Part 1). MICHTOX was developed as a planning tool for the LMMBP using information available at the time to construct a screening-level model for the transport, fate, and bioaccumulation of total PCBs in Lake Michigan. Because of its availability, MICHTOX is now being applied as a tool for the rapid, preliminary assessment of the LMMBP data for PCBs. MICHTOX was previously applied in a similar manner to assess atrazine (Rygwelski *et al*., 1999), another toxic chemical prioritized by the LMMBP. The MICHTOX assessment is, in part, being conducted to generate preliminary modeling results for inclusion in the 2002 Lake Michigan Lake-wide Management Plan (LaMP) Report. This assessment includes comparisons of MICHTOX simulation results to total PCBs concentration data generated by the LMMBP. Such a comparison provides a unique opportunity to confirm the MICHTOX model using data not available at the time of its development. The assessment also compares total PCBs forcing function estimates from the LMMBP to those estimated previously for MICHTOX. In addition, the model was applied to forecast the effectiveness of several toxics management alternatives for PCBs in Lake Michigan. It should be recognized, however, that the preliminary MICHTOX assessment will be superceded in the next several years by mass balance models with significantly better resolution, better process, and better state variable representations. Furthermore, these newer models will be capable of making full use of the LMMBP data; for example, they can be used to model PCBs as individual congeners.

2.4 Description of Model, Data, and Simulations

2.4.1 MICHTOX Model

The MICHTOX model was developed to simulate the transport, fate, and bioaccumulation of PCBs and other toxic chemicals in Lake Michigan. The development and original application of MICHTOX are documented in Part 1 of this report, which includes a thorough description of the model. A schematic diagram of the MICHTOX contaminant transport and fate model is presented in Figure 2.1. Figure 2.2 displays the spatial segmentation of the MICHTOX model, which includes 17 water column segments (divided into epilimnion and hypolimnion segments in the main lake), and seven surficial sediment segments. MICHTOX was implemented using the USEPA WASP4 modeling framework (Ambrose *et al*., 1988) and the Manhattan College food chain model (Version 3.20; Connolly, 1991). The model was originally developed and run on a MicroVax minicomputer and was later modified by the USEPA to run on Compaq (Digital) Alpha OSF1 workstations.

In October 2001, the Great Lakes Environmental Center (GLEC) began resurrection of the MICHTOX source code and input data using Secure Remote Access to connect to the USEPA workstation llrssrv2 over the Internet. All necessary files were identified and reorganized in a user directory, ~dde/MICHTOX/GLEC. The original MICHTOX PCBs simulations were rerun to confirm that the model reproduced the earlier results. Because Secure Remote Access was disrupted in December 2001, it was necessary to move the model to GLEC personal computers for final PCBs simulations. The MICHTOX source code was C preprocessed at LLRS, e-mailed to GLEC, and recompiled using Compaq Visual Fortran 6.1. Results of personal computer simulations were compared to the same simulations run on Alpha workstations, again to confirm that model results were independent of the computer platform.

The goal of this Work Assignment was to rapidly evaluate the LMMBP data for PCBs; therefore, MICHTOX was not significantly revised or recalibrated. However, a number of modifications

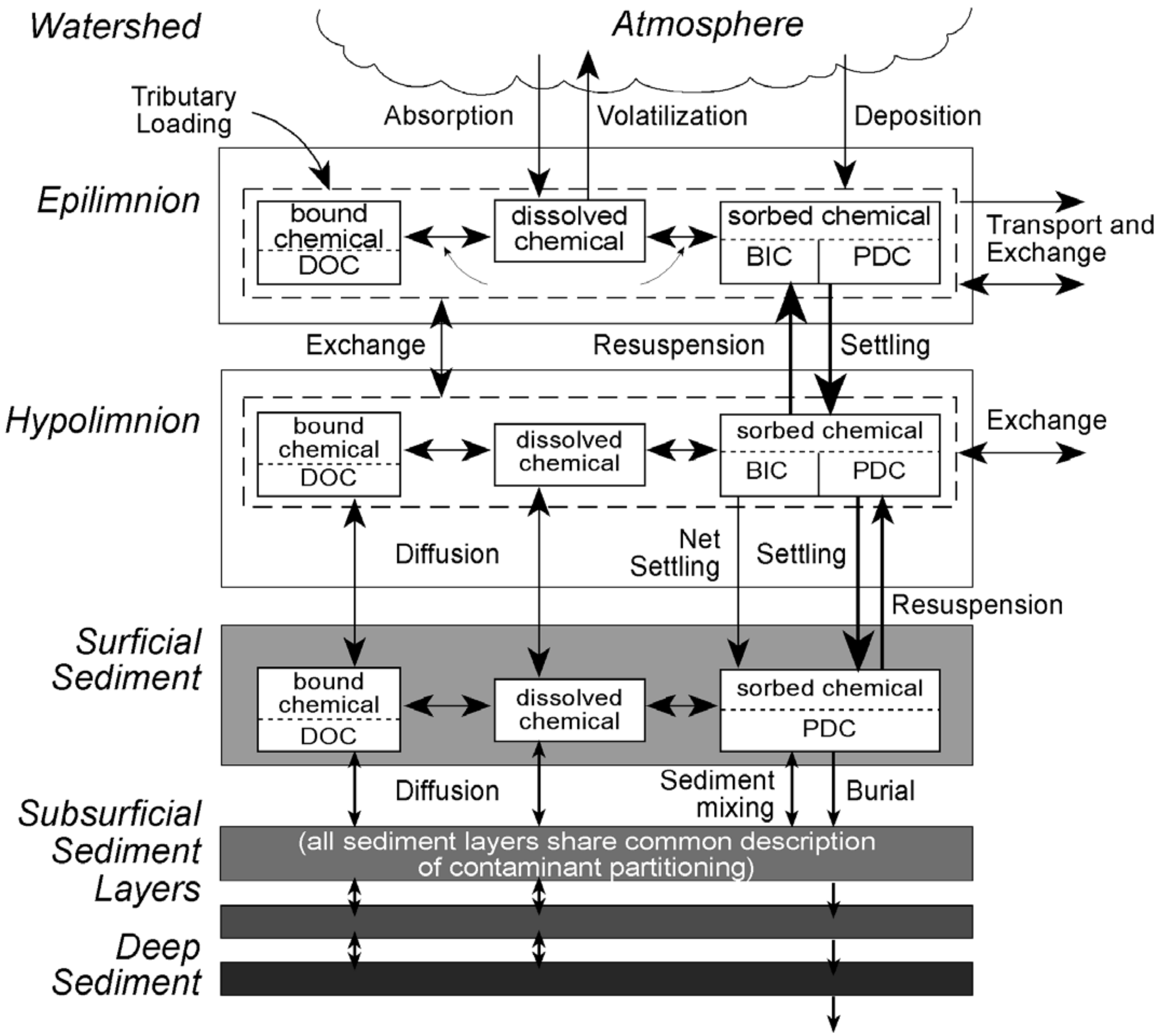

Figure 2.1. MICHTOX mass balance schematic.

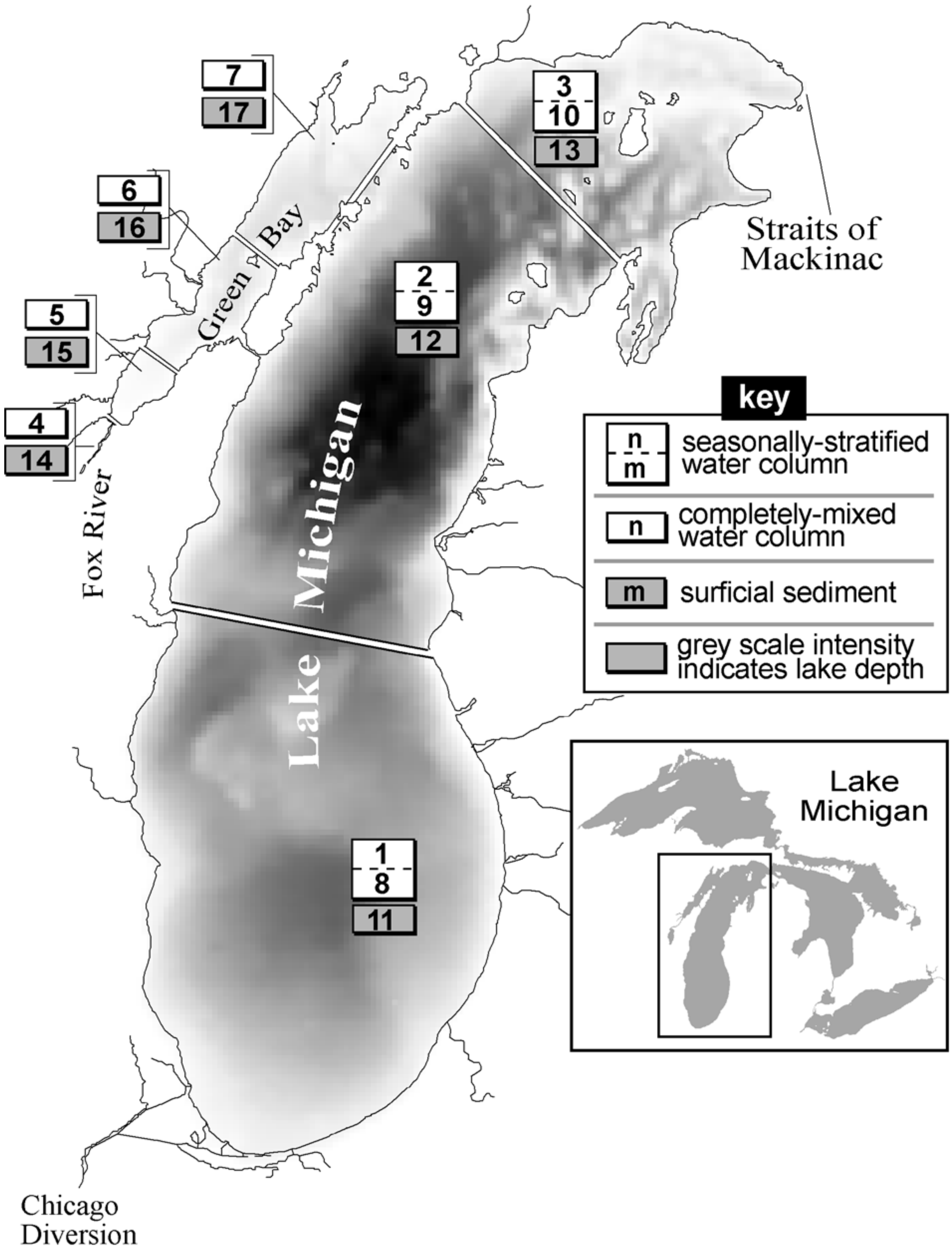

Figure 2.2. Spatial segmentation for the 17 segment MICHTOX model.

were made to the MICHTOX model for this work. These included:

1. Correction of water balance to maintain continuity – The specification of advective flow between water column segments in the model input contained small errors, so that the volume of some segments increased during model simulations, while the volume decreased in other segments. The problem was most severe in Segment 3 (northern lake epilimnion), which lost 1.7% of its volume each year. Consequently, very long (>100 year) MICHTOX simulations aborted, because Segment 3 volumes eventually reached zero. To correct the flows so as to maintain continuity on an annual time scale, small adjustments were made to June surface layer flows, entrainment flows, and southern lake tributary inflows.

2. Treatment of the boundary condition at the Straits of Mackinac – The boundary condition at the Straits of Mackinac was modeled as a seasonally, bidirectional flow. To specify concentrations of model state variables for the reversing flow components, available data, including the LMMBP data, were examined to estimate the concentration gradients across the Straits of Mackinac. The LMMBP total PCBs data for both surface and deepwater samples at Stations MB72M (northern Lake Michigan) and LH54M (northern Lake Huron) suggested that Lake Huron boundary concentrations were about 5% lower than concentrations in northern Lake Michigan. Therefore, boundary concentrations were specified to be 95% of the value simulated for northern Lake Michigan in the previous model time-step. This treatment is consistent with other analyses, such as Robbins (1985) and Thomann and Di Toro (1983), which suggest that similar concentration trends are expected in northern Lake Michigan and Lakes Huron and Superior.

3. Specification of atmospheric vapor concentrations – The model program was modified for the input of atmospheric vapor concentrations as segment-specific forcing functions. Originally, a single forcing function was used for atmospheric vapor concentrations in all MICHTOX surface water segments.

4. Updating of chemical volatilization rate formulations - Revision of the mass transfer formulations used to calculate volatilization rates was recommended by the LMMBP Atmospheric Workgroup. Specifically, the Workgroup recommended the Wanninkhoff (1992) formulation for water mass transfer resistance and the Schwarzenback *et al*. (1993) formulation for gas mass transfer resistence as being the most appropriate for modeling the air-water exchange of PCBs in Lake Michigan. The volatilization rates input to MICHTOX were recalculated on a monthly basis using these formulations. In addition, the subroutine used to calculate chemical volatilization in the LMMBP Level 2 and 3 mass balance models were also modified to include these formulations.

5. Updating parameterization for Henry's constants – Another recommendation of the Atmospheric Workgroup was to make use of recently developed data for the Henry's Law constant for PCBs congeners published by Bamford *et al*. (2000). These data included measurements of Henry's constants at different temperatures. A model which extends these data to the predictions of Henry's constant for all PCBs congeners was obtained (Bamford *et al*., 2002) from the authors. The Bamford model was applied to predict values of Henry's constants for PCBs in MICHTOX, using average monthly surface water temperatures. The Bamford model was also implemented as a spreadsheet and provided to the USEPA for inclusion in the Level 2 and 3 LMMBP mass balance models.

6. Development of an alternative formulation for dispersive water column transport – An alternative formulation for dispersive water column transport was developed for MICHTOX in 1997 (M. Settles, personal communication). This was implemented to replace the original WASP4 mass transport term, which was based on a simple concentration gradient formulation. Tests conducted with both versions of the model indicated that predicted PCBs concentrations were about 15-20% higher in hypolimnetic water column segments in model simulations using the alternative formulation; differences were smaller in other model segments. This modification, intended to address a potential instability in the

model, was apparently never fully tested. Therefore, the original formulation for dispersive water column transport was restored in the version of MICHTOX used for this work.

2.4.2 Mass Balance Data for PCBs

MICHTOX resolves total PCBs (i.e., the sum of congener concentrations) as the sum of two homologs, tetrachlorobiphenyl (PCB4) and pentachlorobiphenyl (PCB5). Although this is technically incorrect (i.e., there are ten homologs), this representation of total PCBs as two homologs was considered a reasonable compromise between pre-LMMBP loading and concentration data, mostly quantified as total PCBs and/or Aroclors, and congener-specific estimates available for physicochemical model parameters.

PCBs concentrations were reported in the LMMBP for some 90 congener peaks; 36 were selected for mass balance modeling based upon their detectability in various media. Forcing functions (atmospheric vapor concentrations, deposition fluxes, and tributary loadings) were also estimated for total PCBs and the selected congeners. Unfortunately, similar estimates were not developed for PCBs homologs. Thus it was necessary to use the total PCBs forcing functions in MICHTOX. Total PCBs forcing functions were evenly split between PCB4 and PCB5 homologs, the same assumption that was made in the original MICHTOX application. It was not possible to confirm this assumption within the time constraints of this project. The total PCBs forcing functions and concentration data are summarized below:

1. <u>Atmospheric vapor concentrations</u> – The LMMBP atmospheric data were used to develop regional spatial and temporal interpolations of PCBs vapor concentrations (Green *et al*., 2000). The 5 km interpolated total PCBs vapor concentrations were averaged on a monthly basis for each MICHTOX surface water segment. The resulting time functions are plotted for the three main lake surface water segments in Figure 2.3. Patterns of both seasonal and spatial variability were evident in the vapor concentration estimates. Because the model predictions of surface water concentrations were found to be sensitive to the monthly variability of PCBs vapor concentrations, this and the other forcing functions were specified on a monthly basis for all MICHTOX simulations.

2. <u>Atmospheric deposition fluxes (wet and dry)</u> – The LMMBP atmospheric data were also used to develop regional spatial and temporal interpolations of PCBs wet and dry deposition fluxes. The deposition fluxes were averaged on a monthly basis and converted into loadings using the surface area of each MICHTOX surface water segment. The resulting time functions for wet and dry deposition are plotted for the southern main lake surface water segment (Segment 1) in Figure 2.4. Estimated deposition fluxes for total PCBs were much higher in 1994, the first year of the LMMBP, due to the enhanced wet deposition flux in the spring of that year.

3. <u>Tributary loadings</u> – Ten Lake Michigan tributaries were monitored during the LMMBP, and the data were used to estimate loadings of toxic chemicals and other constituents to the lake. Tributary loading estimates for total PCBs were summed for each surface water segment, and input to the model as monthly average loadings. The tributary loading time functions for model Segments 1 and 5 are plotted in Figure 2.5; tributary loadings to other segments were very small. As was the case for the other PCBs forcing functions, there was a definite pattern to the seasonal trend of tributary loadings, with highest values estimated in the spring of each year.

4. <u>Water column concentrations</u> – Total PCBs concentrations were averaged for each cruise and water column segment using a volume-weighted averaging (VWA) procedure. Dissolved (filtered) and particulate total PCBs concentrations were averaged separately. Dissolved fraction of total PCBs concentrations are presented in Table 2.1, and particulate concentrations are presented in Table 2.2.

5. <u>Surficial sediment concentrations</u> – Total PCBs concentrations were measured in 133 surficial sediment samples; 50 were collected from the top 1 cm increment of box cores, and 65 were Ponar samples. All total PCBs data were interpolated onto a uniform grid using a natural-neighbor algorithm and then averaged for each

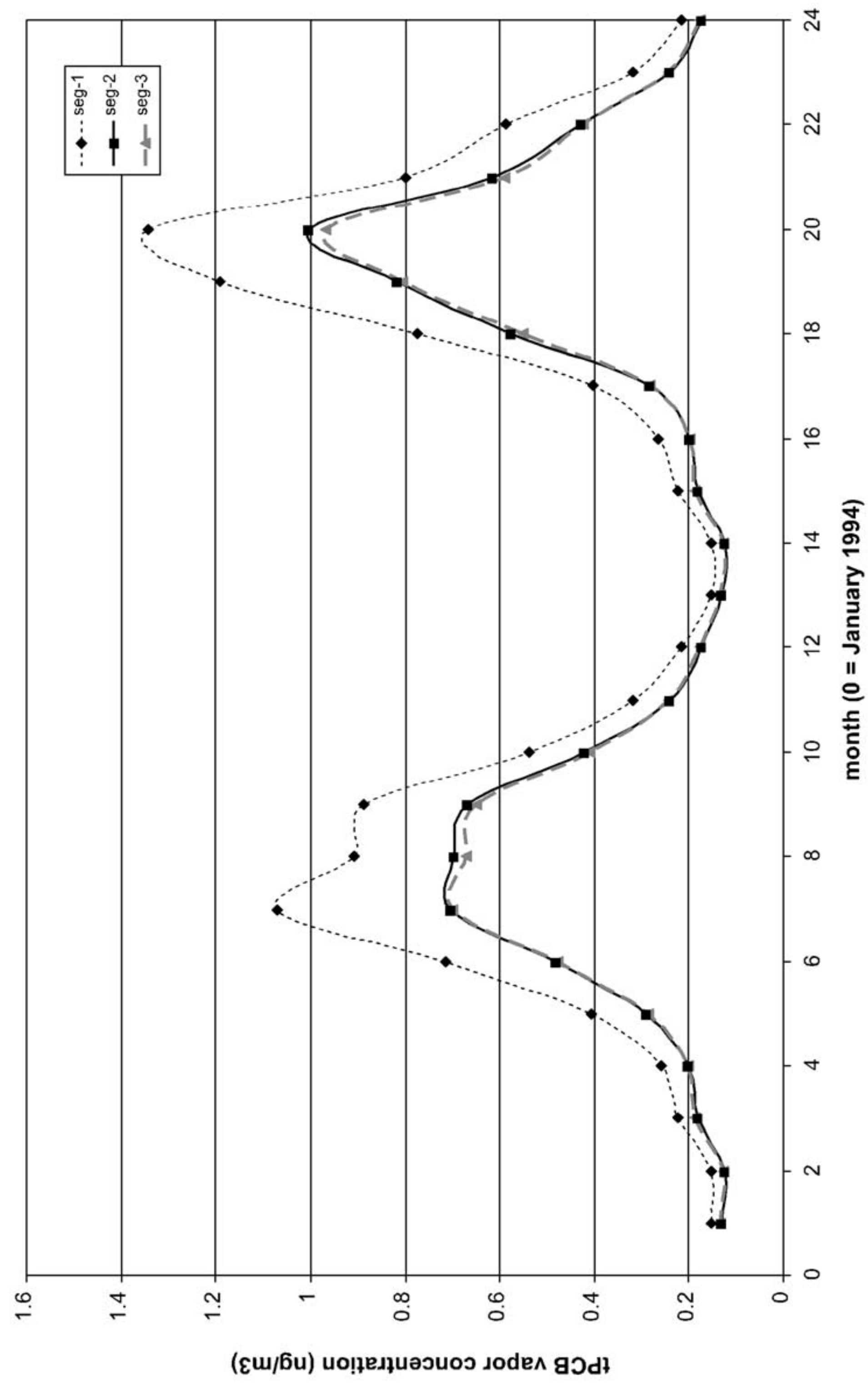

Figure 2.3. The LMMBP estimates of total PCBs atmospheric vapor concentrations processed as monthly values for MICHTOX Segments 1-3.

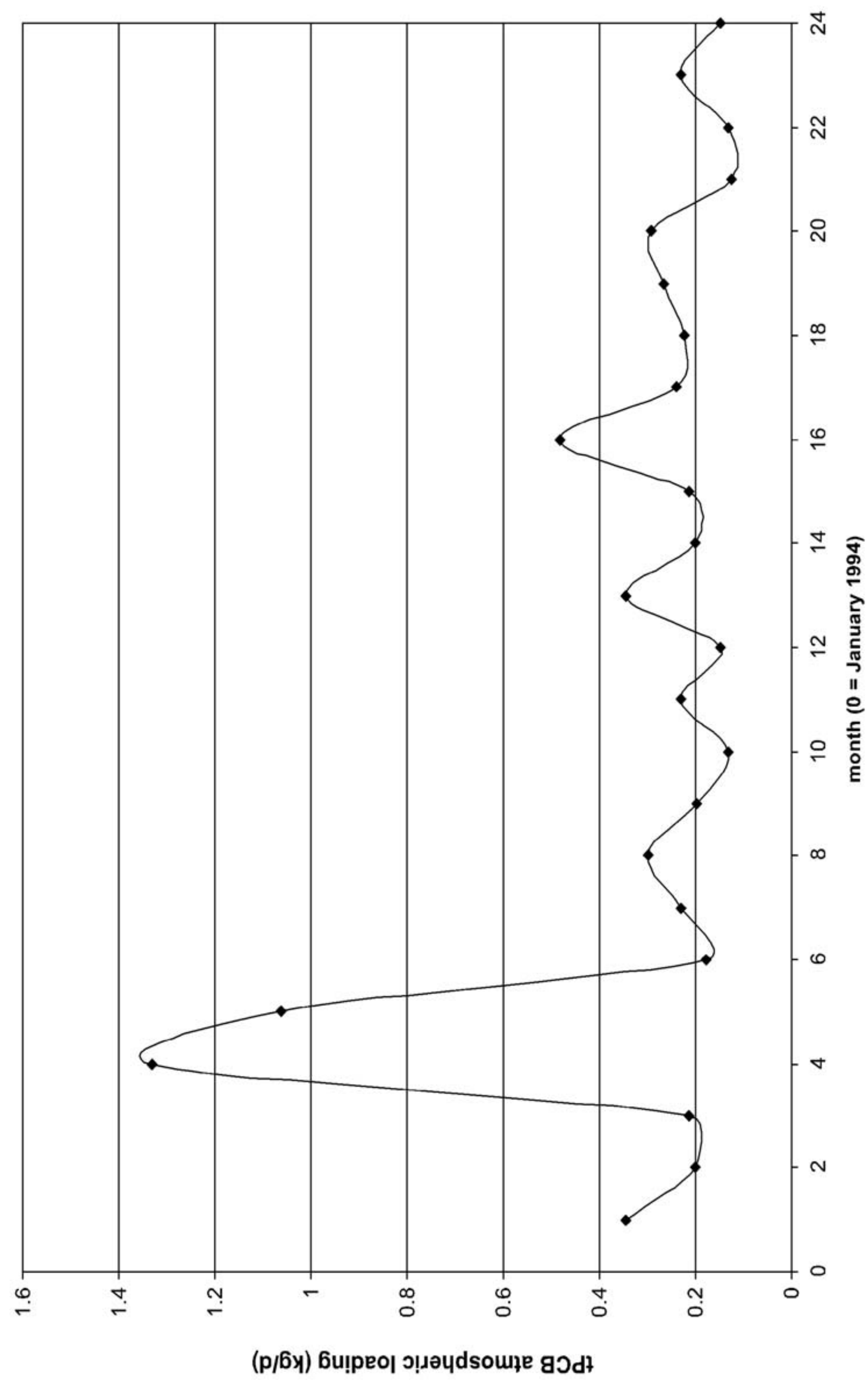

Figure 2.4. The LMMBP estimates of total PCBs atmospheric wet and dry deposition processed as monthly values for MICHTOX Segment 1 (southern Lake Michigan).

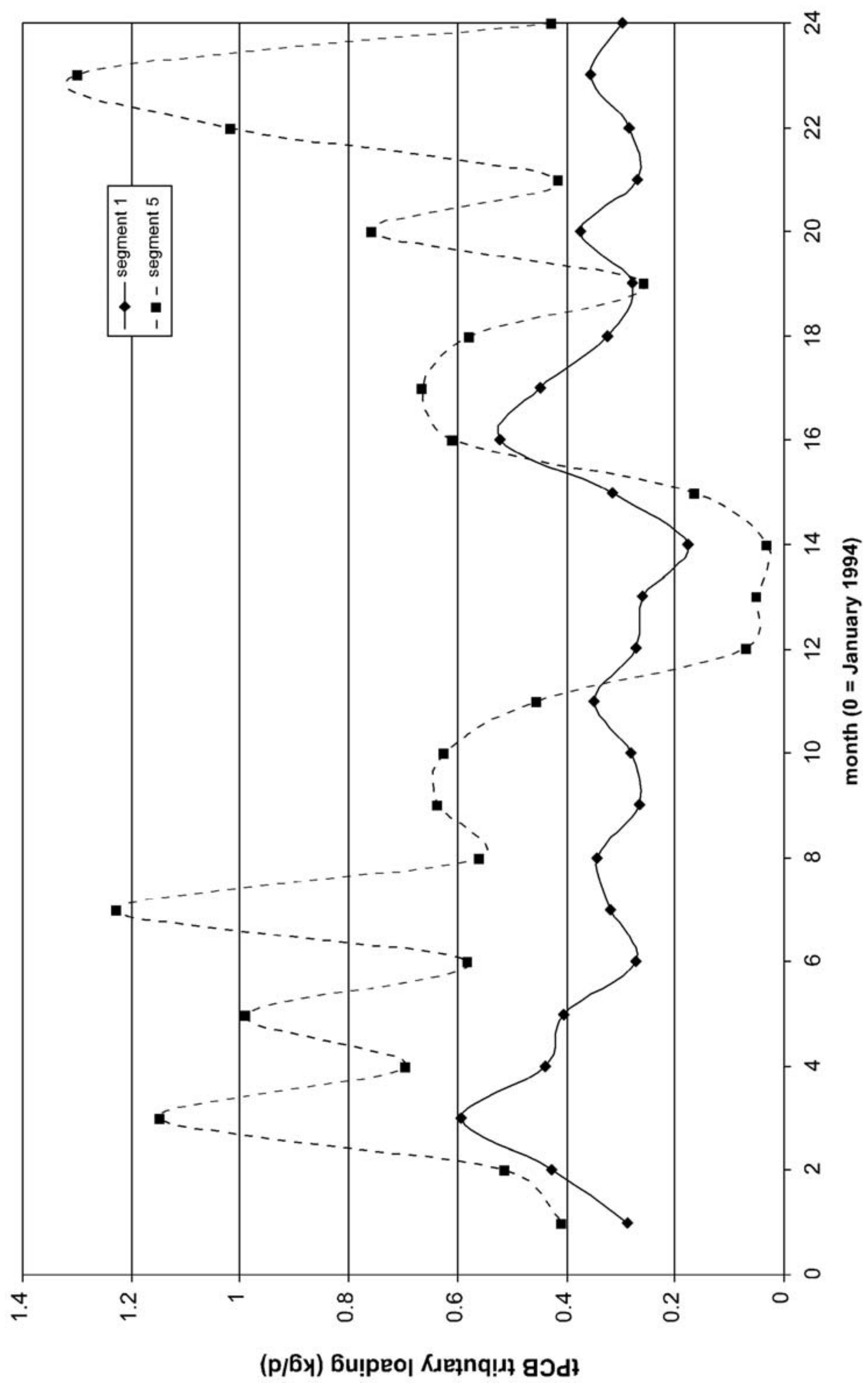

Figure 2.5. The LMMBP estimates of total PCBs tributary loading processed as monthly values for MICHTOX Segment 1 (southern Lake Michigan).

Table 2.1. Cruise- and Segment-Specific Dissolved Fraction of Total PCBs Concentrations (ng/L)

Date	Seg-1	Seg-2	Seg-3	Seg-5	Seg-6	Seg-7	Seg-8	Seg-9	Seg-10
May-94	0.53	0.51	0.35	0.36	0.36	0.36	0.54	0.50	0.34
Jun-94	0.59	0.64	0.61				0.59	0.60	0.58
Aug-94	0.85	0.85	0.84	0.50	0.49	0.77	0.69	0.75	0.75
Oct-94	0.67	0.81	0.83	0.40	0.40	0.61	0.68	0.81	0.84
Jan-95	0.54	0.54	0.54						
Apr-95	0.66	0.68	0.66	0.36	0.37	0.49	0.66	0.67	0.66
Aug-95	0.82	0.86	0.88	0.74	0.74	0.74	0.71	0.79	0.81
Sep-95	0.87	0.88	0.87	0.31	0.31	0.53	0.83	0.87	0.87

Table 2.2. Cruise- and Segment-Specific Average Particulate Total PCBs Concentrations (ng/L)

Date	Seg-1	Seg-2	Seg-3	Seg-5	Seg-6	Seg-7	Seg-8	Seg-9	Seg-10
May-94	0.147	0.137	0.132	1.653	1.659	0.272	0.114	0.120	0.123
Jun-94	0.088	0.065	0.071				0.090	0.070	0.072
Aug-94	0.031	0.030	0.024	0.574	0.577	0.103	0.080	0.055	0.045
Oct-94	0.102	0.042	0.030	0.608	0.598	0.121	0.099	0.045	0.030
Jan-95	0.138	0.136	0.138						
Apr-95	0.099	0.084	0.075	0.805	0.789	0.245	0.089	0.073	0.071
Aug-95	0.046	0.026	0.025	0.048	0.050	0.064	0.111	0.058	0.050
Sep-95	0.036	0.023	0.020	0.572	0.571	0.126	0.052	0.026	0.025

MICHTOX surficial sediment segment. Average total PCBs concentrations were also calculated for the box core samples in each main lakesediment segment (Segments 11-13). Relatively few sediment samples were collected in Green Bay. Thus surficial sediment total PCBs concentrations measured in box cores collected during the 1989-1990 Green Bay Mass Balance Project (GBMBP) were used to calculate average concentrations in Green Bay sediment (Segments 15-17). Segment-specific average total PCBs sediment concentrations are presented in Table 2.3.

According to the LMMBP Quality Assurance Project Plan (QAPP), samples from deeper intervals in selected sediment cores were to be analyzed for PCBs in addition to the 0-1 cm interval. However, these data were not available at the time of this report.

6. Biota concentrations – Fish and lower food chain organisms were sampled in three biota zones. Two of the zones, Saugatuck and Sheboygan Reef, fall within the southern lake basin (Segments 1/8). A third zone, Sturgeon Bay, is located in the northern lake basin (Segments 2/9). It should be noted that there was some confusion regarding the identification of biota samples from Saugatuck and Sturgeon Bay in the database from which these data were retrieved. Although GLEC believes that the data have now been associated correctly with biota zones, this has not been confirmed by the USEPA. Although biota sampling was conducted on a seasonal basis, all samples were averaged for use with MICHTOX. Total PCBs concentrations measured in the three biota zones, based on age or size classes, are presented in Table 2.4(a-c).

Table 2.3. Segment-Specific Average Surficial Sediment Total PCBs Concentrations (ng/g)

Segment	All LMMBP Surficial Sediment Samples	Surficial Samples From LMMBP Box Cores	Surficial Samples From GBMBP Box Cores
11	56.2	102	
12	35.2	63.4	
13	4.99	27.9	
15	17.1		695
16	127		643
17	52.9		97.3

Table 2.4a. Average Total PCBs Concentrations in Fish in the Saugatuck Biota Zone

Species	Age (Years)	Average PCBs Concentrations (ng/g)	PCBs Standard Deviation (ng/g)
Alewife < 120 mm	1-2	304	167
Alewife > 120 mm	3-7	592	140
Bloater < 160 mm	1-3	586	201
Bloater > 160 mm	4-7	875	250
Deepwater Sculpin	4+	340	101
Lake Trout	1	175	
Lake Trout	2	904	171
Lake Trout	3	883	288
Lake Trout	4	1287	241
Lake Trout	5	2068	532
Lake Trout	6	3185	1126
Lake Trout	7	3609	809
Lake Trout	8	4511	921
Lake Trout	9	5728	1645
Lake Trout	10	8209	4101
Lake Trout	11	7477	2515
Lake Trout	12	8116	2997
Lake Trout	13	6666	872
Lake Trout	14	6799	794
Lake Trout	15	4014	3268
Smelt (Adult)	1-7	294	69
Slimy Sculpin	1-6	390	149

Table 2.4b. Average Total PCBs Concentrations in Fish in the Sheboygan Reef Biota Zone

Species	Age (Years)	Average PCBs Concentrations (ng/g)	PCBs Standard Deviation (ng/g)
Alewife < 120 mm	1-2	347	211
Alewife > 120 mm	3-7	540	106
Bloater < 160 mm	1-3	753	132
Bloater > 160 mm	4-7	876	148
Deepwater Sculpin	4+	427	90
Lake Trout	3	547	184
Lake Trout	4	706	217
Lake Trout	5	1202	204
Lake Trout	6	1395	192
Lake Trout	7	1974	320
Lake Trout	8	2668	1001
Lake Trout	9	3102	1022
Lake Trout	11	5322	1215
Lake Trout	12	4692	1234
Lake Trout	13	4466	217
Lake Trout	14	3483	
Smelt (Adult)	1-7	305	133

Table 2.4c. Average Total PCBs Concentrations in Fish in the Sturgeon Bay Biota Zone

Species	Age (Years)	Average PCBs Concentrations (ng/g)	PCBs Standard Deviation (ng/g)
Alewife < 120 mm	1-2	170	71
Alewife > 120 mm	3-7	589	171
Bloater < 160 mm	1-3	604	155
Bloater > 160 mm	4-7	739	189
Deepwater Sculpin	4+	325	59
Lake Trout	1	350	163
Lake Trout	2	395	107
Lake Trout	3	889	159
Lake Trout	4	1268	270
Lake Trout	5	1707	309
Lake Trout	6	2487	577
Lake Trout	7	2656	509
Lake Trout	8	3360	559
Lake Trout	9	4211	757
Lake Trout	10	5283	1168
Lake Trout	11	5939	1543
Lake Trout	12	4420	1185

2.4.3 Revised MICHTOX and LMMBP Forcing Functions

New total PCBs forcing functions were developed for the MICHTOX simulations presented in this report. As mentioned previously, these forcing functions included: atmospheric vapor concentrations, atmospheric (wet and dry) deposition loadings, and tributary loadings. The new total PCBs forcing functions were based upon the LMMBP estimates presented previously in conjunction with other information regarding long-term trends in PCBs usage, loadings, and concentrations in Lake Michigan and the Great Lakes. This latter information was used to develop the continuous total PCBs forcing functions necessary to run the MICHTOX simulation from an uncontaminated initial condition. It is important to consider trends in long-term loads and other forcing functions. These relate directly and indirectly to chemical transport and fate over comparable time scales. Other simulations were conducted with MICHTOX to predict the effectiveness of several toxic chemical management scenarios.

The forcing functions developed for PCBs by the LMMBP are believed to be accurate estimates for the 1994-1995 period, based upon the data quality objectives and well-developed estimation procedures. A number of sources of information were available to characterize trends of the usage and release of PCBs in the Great Lakes during the 20th Century, and these were used to extrapolate the LMMBP forcing functions both backwards and forwards in time. Although somewhat speculative, a similar procedure had been demonstrated for PCBs in Lake Ontario (Mackay, 1989; Gobas *et al*., 1995). The procedure requires the following information:

1. The date when contamination begins.
2. The rate of increase in the magnitude of the forcing function.
3. The date and duration of the loading/forcing function peak.
4. The rate of decline in the magnitude of the forcing function.

Rates of change in vapor phase PCBs concentrations for Lake Michigan and the Great Lakes region have been published by a number of researchers (Hillery *et al*., 1997,1998; Baker and Eisenreich, 1990; Green *et al*., 2000; Schneider *et al*., 2001). Although there is some disagreement as to whether atmospheric measurements support the notion that vapor PCBs concentrations are declining over Lake Michigan, Schneider *et al.* (2001) indicated that PCBs concentration profiles in highly-resolved sediment cores from Grand Traverse Bay support the view that vapor phase PCBs concentrations have been declining at a rate of about 0.115/year, which corresponds to a six-year half-life over the past 25 years.

Similarly, rates of change in PCBs tributary loadings can be determined from loading estimates based upon measurements from the Fox River (in 1989-1990 by Velleux and Endicott, 1994 and in 1994-1995 by the LMMBP) and major tributaries throughout the Lake Michigan basin (in 1982 by Marti and Armstrong, 1990 and in 1994-1995 by the LMMBP). This information yields estimates for the rate of decline in tributary loadings of 0.053 to 0.054/year, corresponding to a 12- to 13-year half-life.

To complete the long-term total PCBs forcing functions, a number of other assumptions were made:

1. PCBs contamination of Lake Michigan commenced in 1940.
2. The rate of increase in vapor concentrations and tributary loadings was the same as the rate of decline.
3. Atmospheric deposition loadings followed the same long-term trends as vapor concentrations.
4. Monthly variability in the magnitude of forcing functions followed the 24-month pattern established by the LMMBP estimates.

The date and duration of the peak in the PCBs forcing functions was not so easily defined. Schneider *et al*. (2001) suggested that forcing functions peaked in 1970, and declined with the decline in chemical production after 1972. On the other hand, Gobas *et al.* (1995) estimated that PCBs loading to Lake Ontario peaked much earlier, in 1961. Why there would be such a difference between Lakes Michigan and Ontario is not clear, and perhaps it reflects the subjectivity of these estimates. Ultimately, three different estimates for long-term total PCBs forcing functions were developed:

1. Scenario A – Total PCBs forcing functions peak in 1970 and decline after 1972.

2. Scenario B – Total PCBs forcing functions peak in 1961 and decline after 1963.

3. Scenario C – Total PCBs forcing functions peak in 1961 and decline after 1972.

Plots of the three forcing function scenarios are provided on a whole-lake basis for vapor concentrations (Figure 2.6), atmospheric deposition (Figure 2.7), and tributary loading (Figure 2.8). In each plot, the forcing function estimate used in the original MICHTOX application are also presented.

Forecast simulations using LMMBP data to define initial conditions for PCBs and alternative forcing functions (representing general toxic chemical management alternatives) using those measured by the LMMBP as a baseline included:

1. No-Change – Total PCBs vapor concentrations, deposition fluxes, and tributary loadings continue in the future at the levels estimated by the LMMBP for 1994-1995.

2. No-Action – Total PCBs deposition fluxes and tributary loadings continue in the future at levels estimated by the LMMBP; however, atmospheric vapor concentrations decline in the future at a rate equal to the observed rate of decline over the past 25 years. This assumes that PCBs vapor concentrations are declining due to the slow depletion of regional-scale inventories (e.g., transformers, contaminated soil, landfills, sewage sludge, etc.) from which PCBs evaporate and act as sources to the atmosphere. It is not clear to what extent these declines may be related to toxic chemical management.

3. Fifty-Percent Function Reduction – Total PCBs vapor concentrations, deposition fluxes, and tributary loadings are reduced from LMMBP 1994-1995 levels by 50% at the start of 2002.

4. Fifty-Percent Reduction – Deposition fluxes and tributary loadings are reduced from LMMBP 1994-1995 levels by 50% at the start of 2002. Total PCBs vapor concentrations continue in the future at the levels estimated by the LMMBP for 1994-1995. In other words, this simulation assumes that vapor concentrations are not controllable.

5. Elimination – Total PCBs vapor concentrations, deposition fluxes, and tributary loadings are eliminated at the start of 2002.

Twenty-year forecasts, simulating the period 1994 through 2014, were made with MICHTOX for each of these toxics management alternatives.

2.5 Results and Discussion

2.5.1 Confirmation of MICHTOX PCBs Bioaccumulation Predictions

Initially, predictions of total PCBs bioaccumulation were made by running the MICHTOX food web model to steady-state, using the average dissolved and particulate total PCBs concentrations observed during the LMMBP in southern Lake Michigan. This was done to separate the bioaccumulation predictions from the transport/fate predictions of the model, which were used in other model runs to define chemical exposure. The bioaccumulation predictions were then compared to average total PCBs concentrations in fish from the Saugatuck and Sheboygan Reef biota zones. These comparisons are plotted in Figures 2.9 and 2.10. MICHTOX consistently underpredicts PCBs bioaccumulation in all fish from Saugatuck, except bloater (Figure 2.9). Model predictions are much more consistent with data for PCBs concentrations in fish from Sheboygan Reef (Figure 2.10), although the model again tends to underpredict PCBs bioaccumulation for older age classes of lake trout. Differences in PCBs concentrations measured in fish at these two locations most likely reflect different local PCBs exposures; sediment PCBs concentrations, for

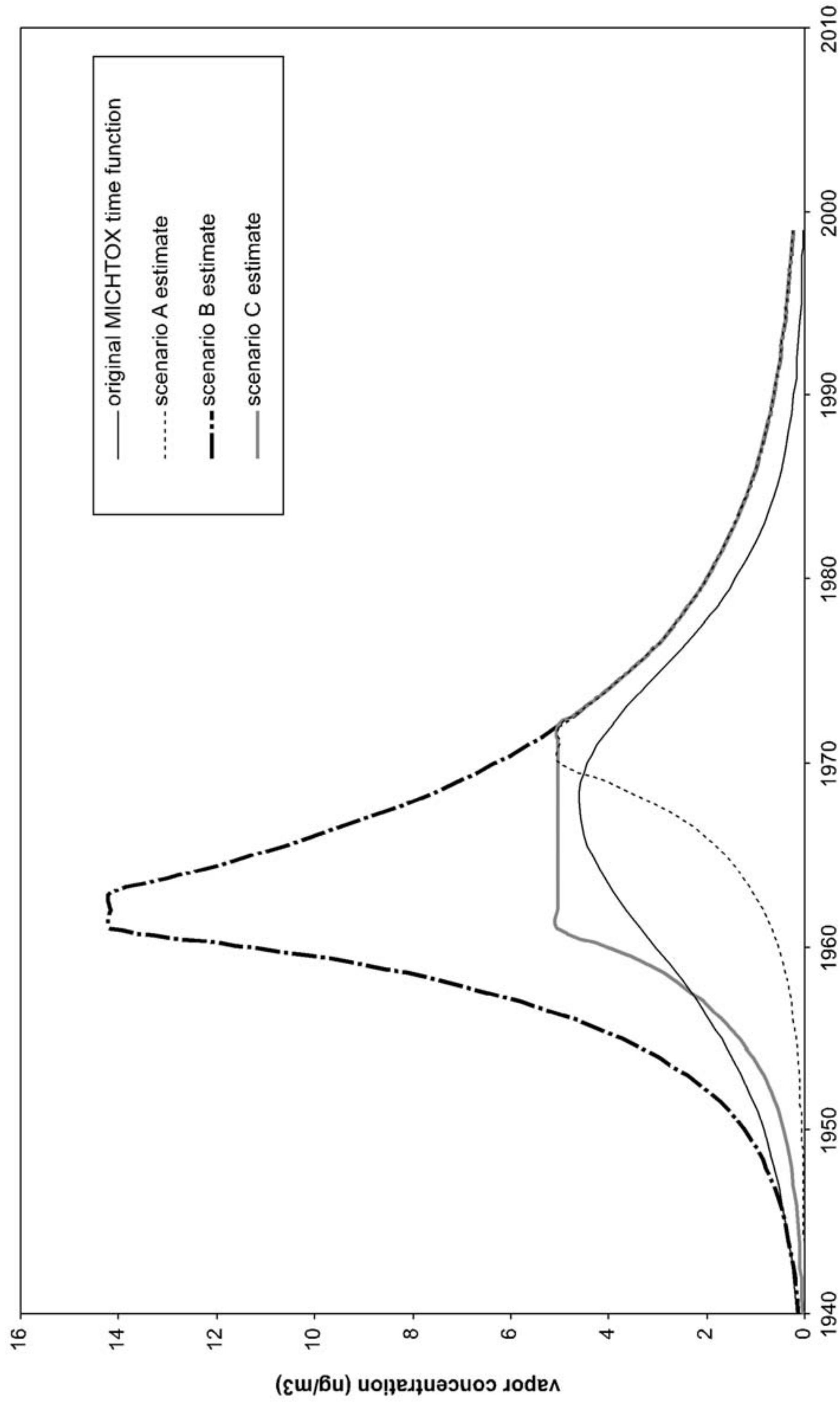

Figure 2.6. Long-term estimates of Lake Michigan total PCBs vapor concentrations.

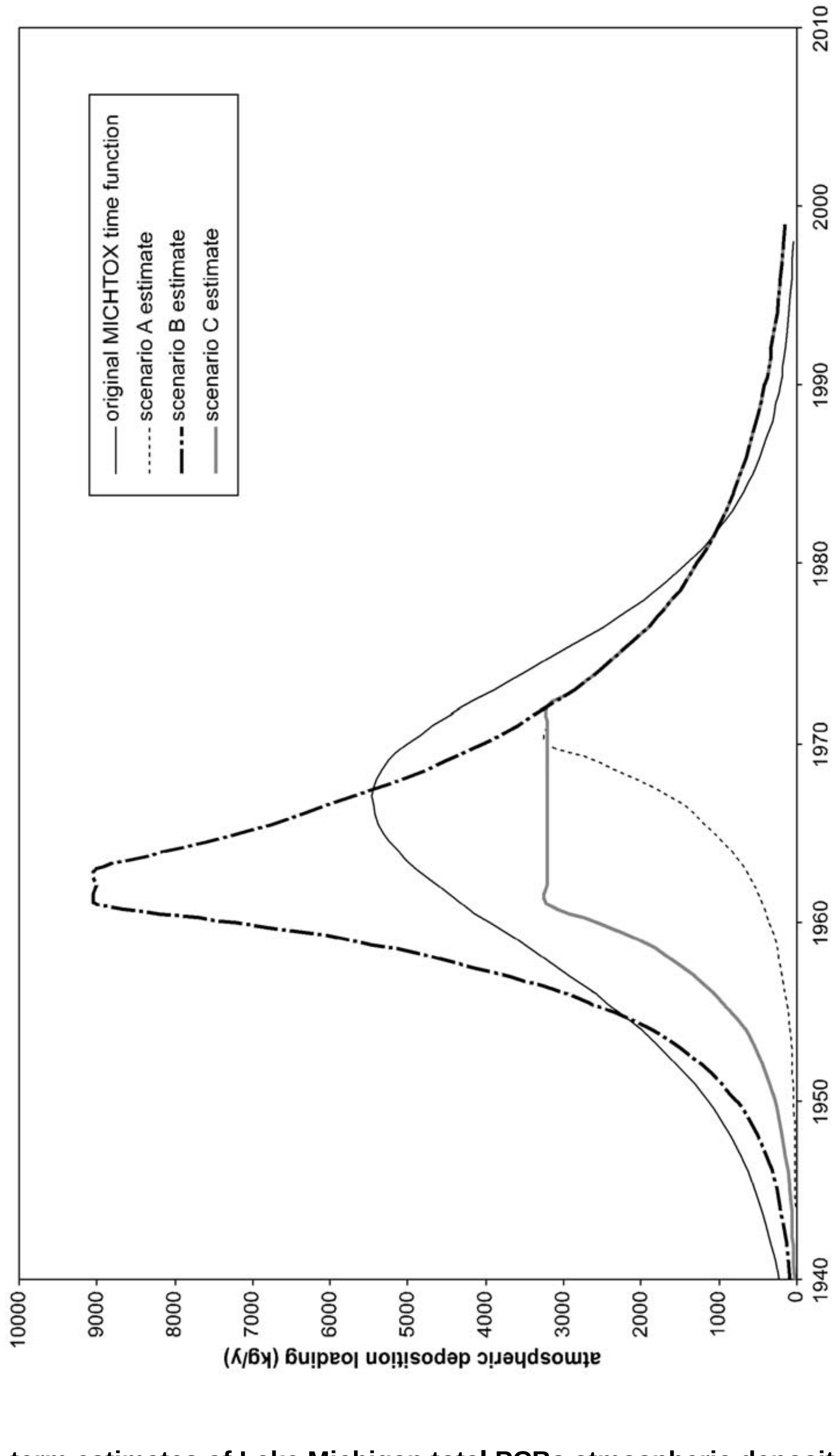

Figure 2.7. Long-term estimates of Lake Michigan total PCBs atmospheric deposition loading.

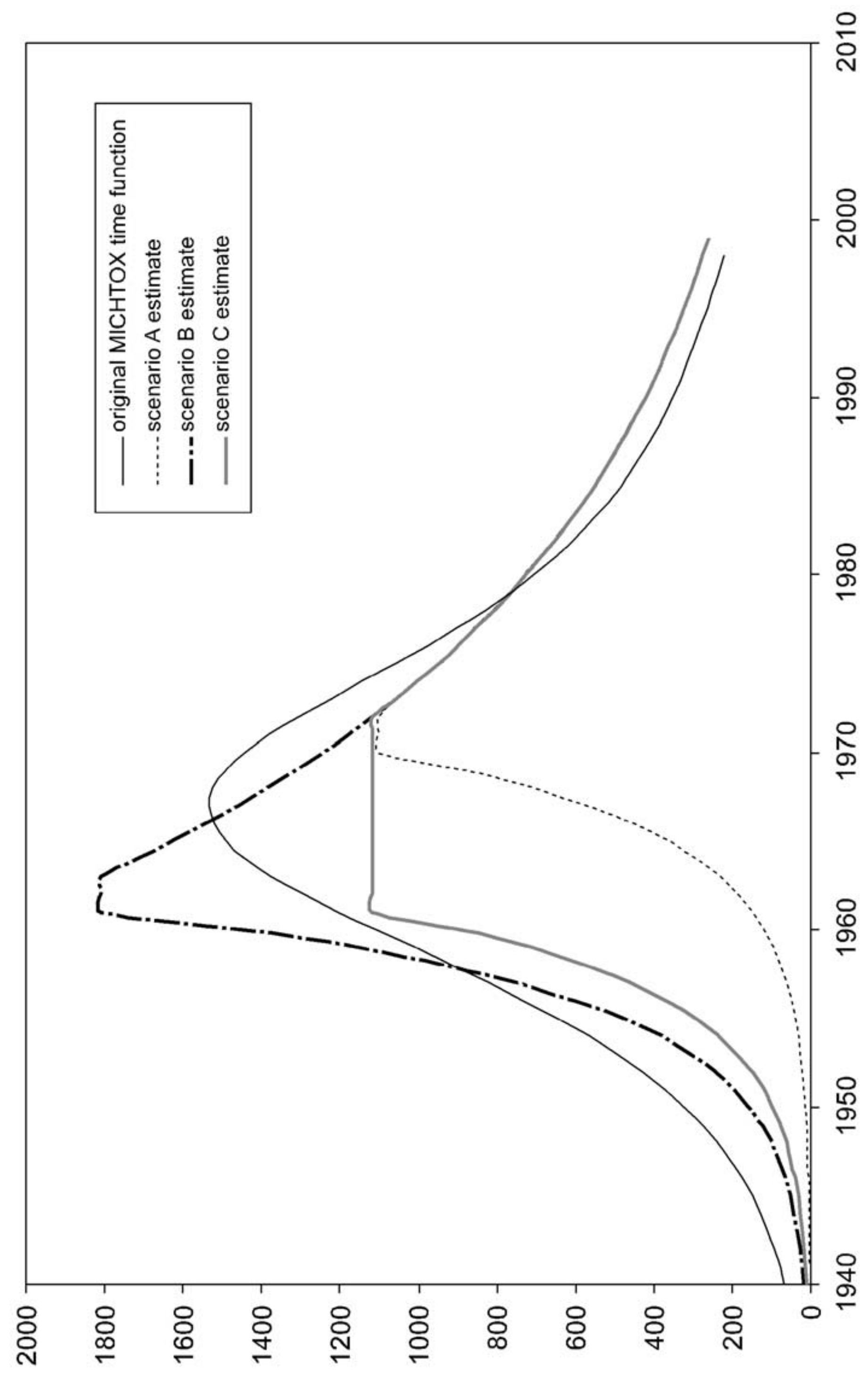

Figure 2.8. Long-term estimates of Lake Michigan total PCBs tributary loading.

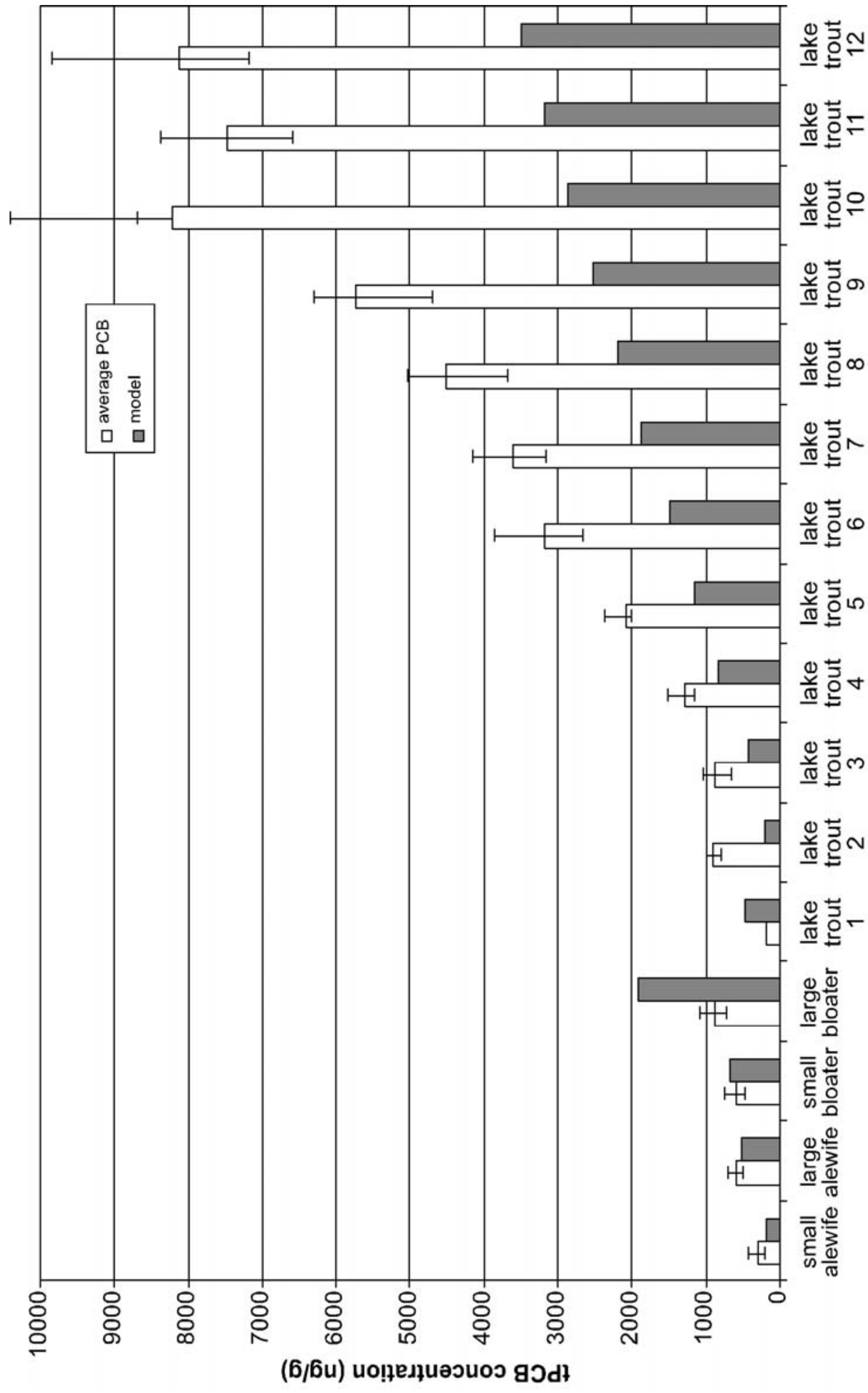

Figure 2.9. Comparison of MICHTOX steady-state total PCBs concentrations to Saugatuck fish data (error bars denote first and third quartiles).

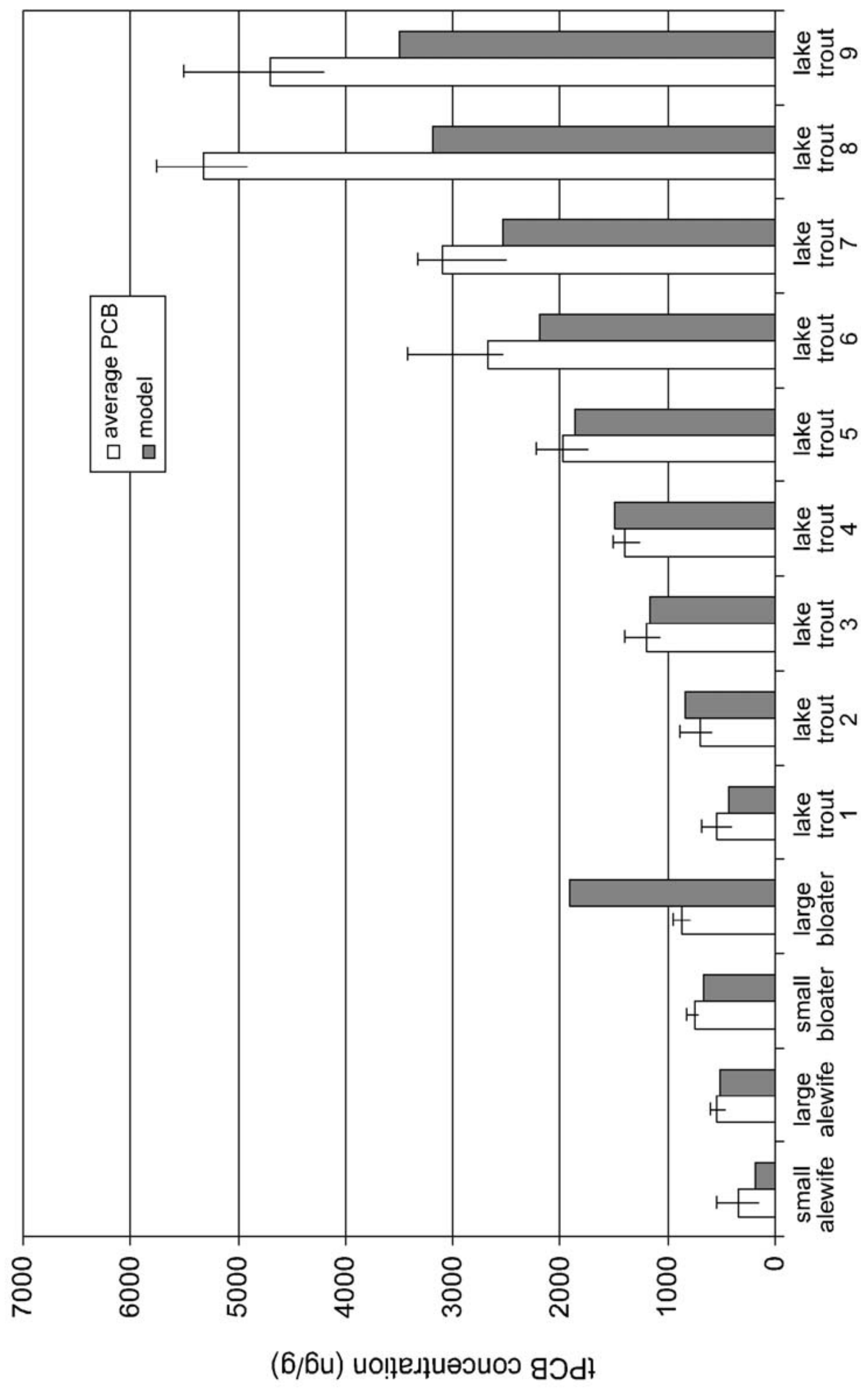

Figure 2.10. Comparison of MICHTOX steady-state total PCBs concentrations to Sheboygan Reef fish data (error bars denote first and third quartiles).

example, are substantially higher at Saugatuck than at Sheboygan Reef. Because both biota zones fall within the same southern Lake Michigan model segment, differences in PCBs exposure concentrations are not reflected in the bioaccumulation model results. Differences in PCBs bioaccumulation may also result from regional variation in trophic dynamics or bioenergetics; LMMBP data characterizing these factors were not examined for this project. The sensitivity of bioaccumulation model predictions are specifically addressed later in Section 2.3.10 of this report.

2.5.2 Comparison of Original MICHTOX PCBs Simulations to the LMMBP Data

The next step taken in the evaluation of the MICHTOX model was to compare PCBs forcing functions (i.e., atmospheric vapor concentrations, atmospheric deposition fluxes, and tributary loadings) used in the original model to estimates generated by the LMMBP. The original and the LMMBP forcing functions for total PCBs are compared on a whole-lake basis for years 1994-1995 in Table 2.5. The LMMBP estimates for atmospheric deposition and tributary loading are reasonably close to the original MICHTOX forcing functions; the original forcing functions are both about 30% lower than the LMMBP estimates. However, the discrepancy is much greater for vapor concentrations; the average total PCBs vapor concentration estimated by the LMMBP is 4.5 times higher than the original MICHTOX value. This discrepancy is much greater than expected, and results from the lack of adequate data available to define lake-wide average PCBs vapor concentrations in the original MICHTOX model. Given the model's sensitivity to vapor concentrations, it was determined that all PCBs forcing functions should be updated based upon the LMMBP estimates, and that these forcing functions should be used to rerun all MICHTOX simulations.

Prior to rerunning the model with the revised forcing functions, the original MICHTOX model predictions of PCBs concentrations in water, sediment, and fish were compared to concentrations measured in the LMMBP. These comparisons are presented in Figures 2.11-2.14. MICHTOX predictions of total PCBs concentrations in main Lake Michigan segments are compared to available water column measurements (including those from the LMMBP) in Figure 2.11. Predictions made with the original model (although referred to as the "original MICHTOX model" in this section, the simulations are based on a version of the model which incorporated the continuity balance and Straits of Mackinac boundary condition modifications discussed previously) appear to be quite consistent with the data over the past 25 years. Predictions of surficial sediment total PCBs concentrations made using the original MICHTOX model are compared to data from three Lake Michigan sediment core profiles in Figure 2.12. Data from these sediment cores, collected by the USEPA Great Lakes National Program Office (GLNPO) in 1991-1992, were used because no sediment cores were analyzed for PCBs in the LMMBP. The agreement between predictions and data is not very satisfactory. In part this is because the transformation of sediment core data from depth intervals to dates was done based upon sedimentation rates, without consideration of the effects of sediment mixing in the surface layers.

Table 2.5. Comparison of Original MICHTOX Total PCBs Forcing Functions for 1994-1995 to the LMMBP Estimates (Whole-Lake Average)

Forcing Function	Original MICHTOX	LMMBP Estimate
Atmospheric Vapor Concentration (ng/m^3)	0.092	0.41
Atmospheric Deposition (kg/y)	151	232
Tributary Loading (kg/y)	261	346

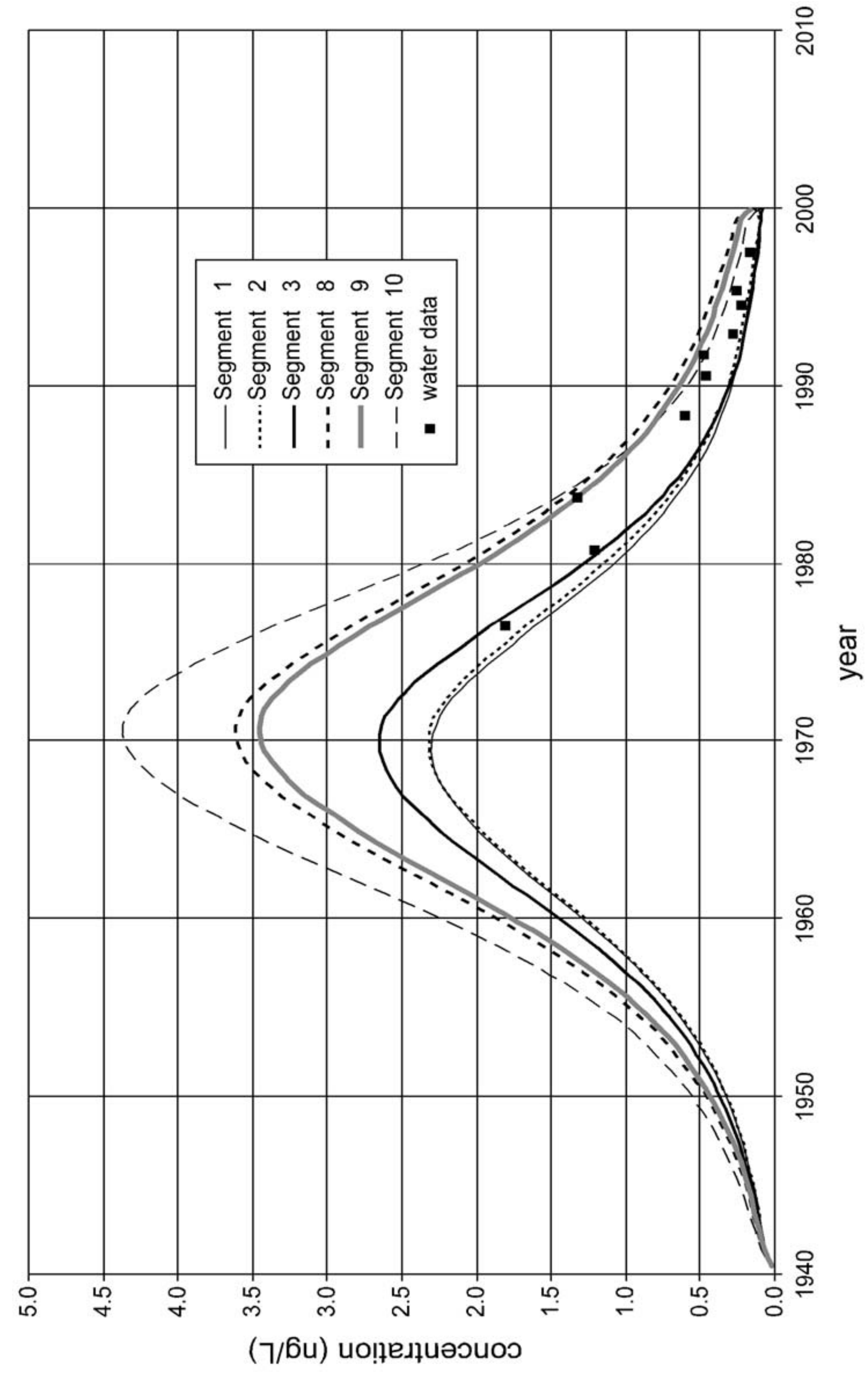

Figure 2.11. Original MICHTOX predictions and data for main lake total PCBs concentrations.

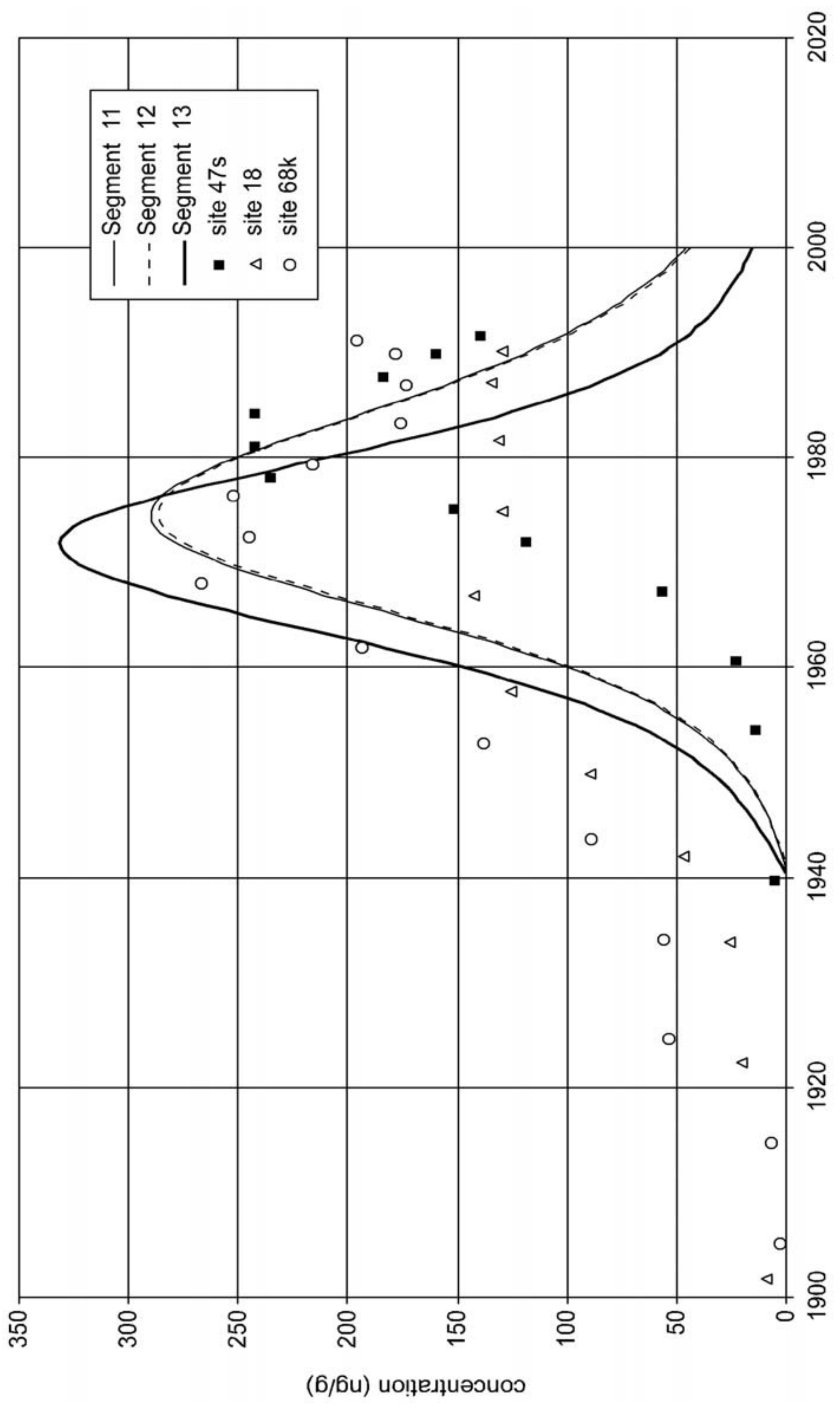

Figure 2.12. Original MICHTOX predictions and data for main lake sediment total PCBs concentrations (sediment cores collected in 1991-1992).

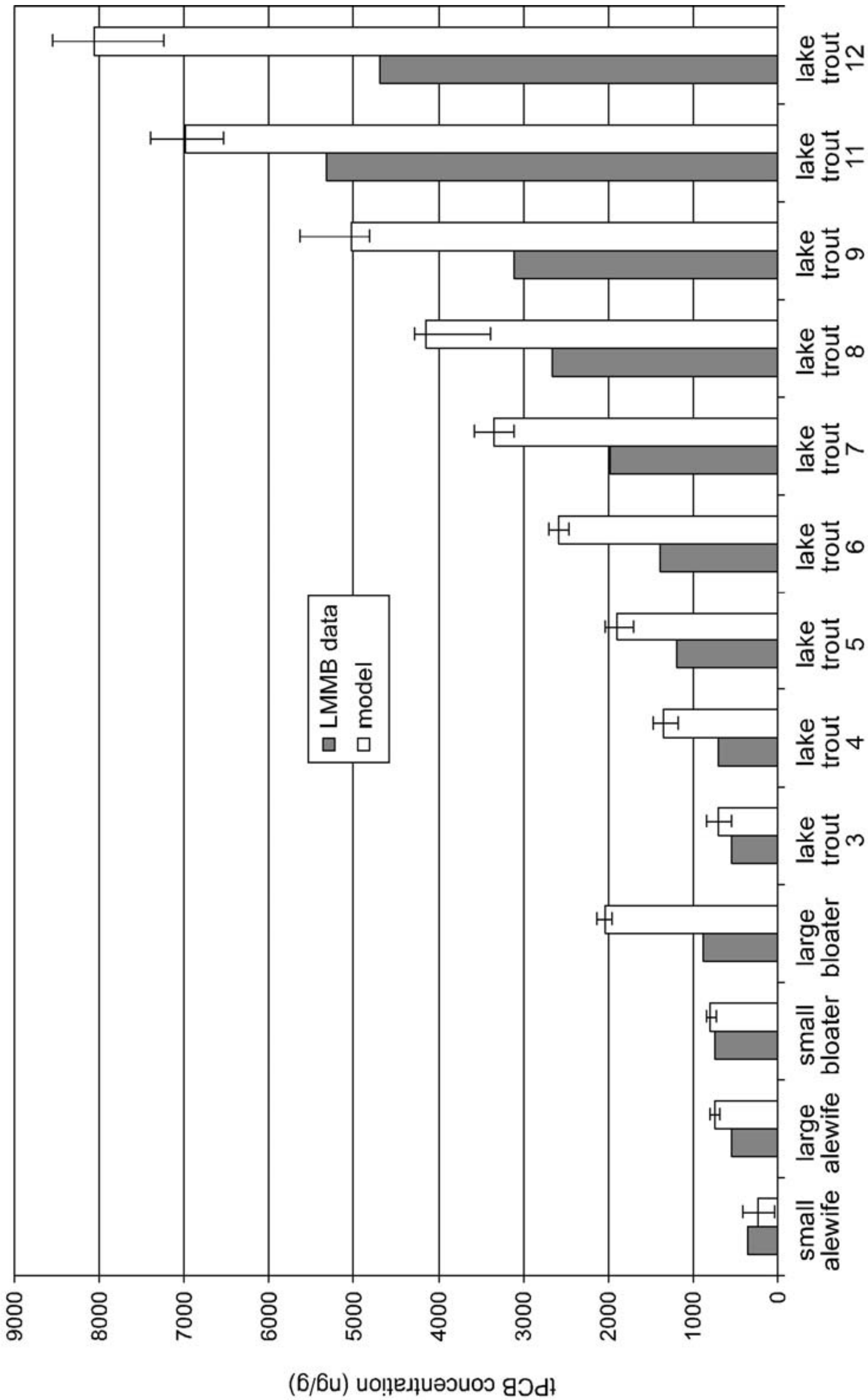

Figure 2.13. Original MICHTOX predictions of total PCBs concentrations in fish and comparison to Sheboygan Reef zone data.

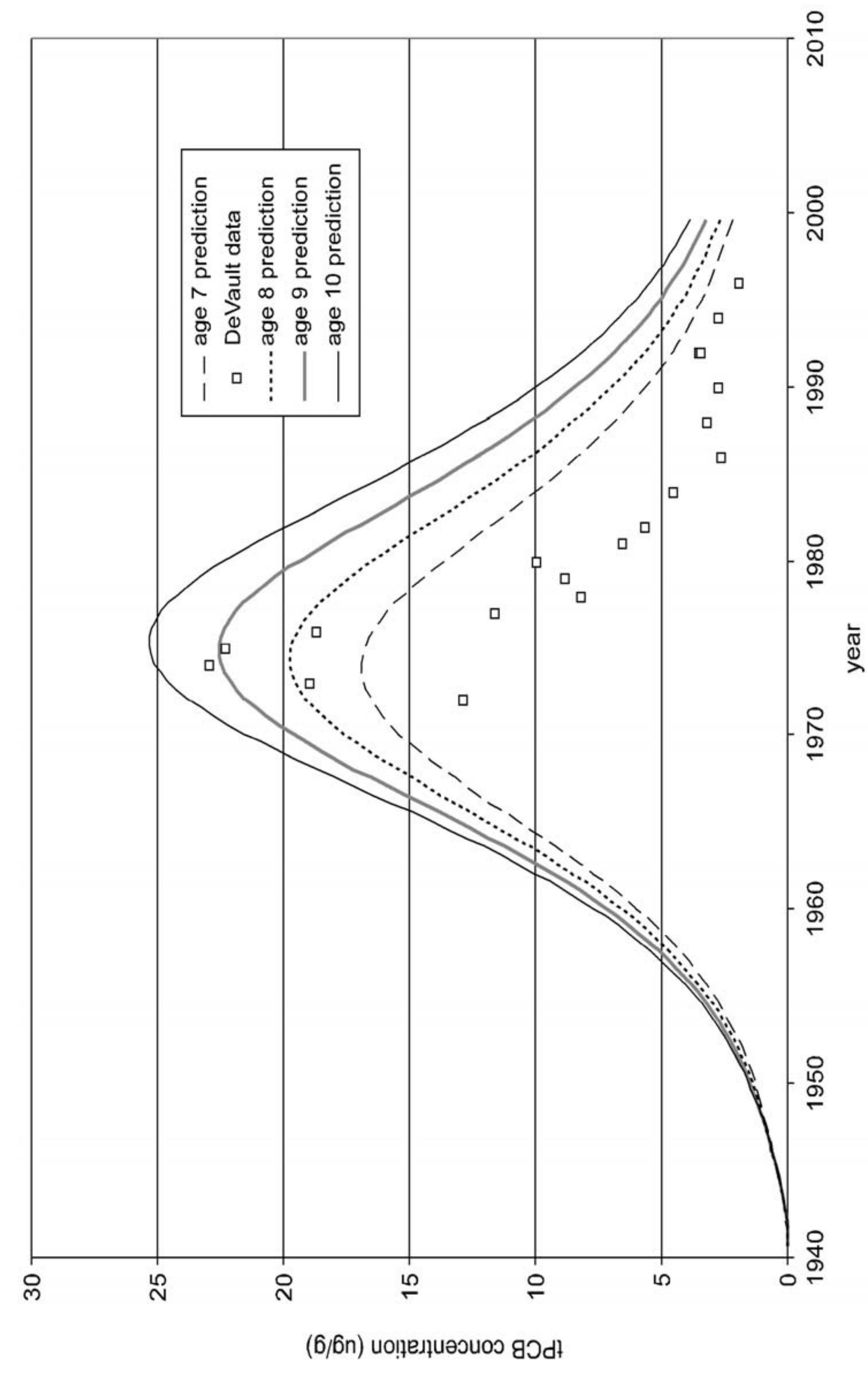

Figure 2.14. Original MICHTOX predictions of total PCBs concentrations in lake trout and comparison to DeVault *et al*. (1986) data.

MICHTOX predictions of total PCBs concentrations in fish are compared to concentration data for fish collected at Sheboygan Reef in Figure 2.13. The observed trend of increasing total PCBs concentrations with fish size and age is captured by the model predictions, although the original model consistently tends to overpredict bioaccumulation in fish at Sheboygan Reef. This tendency for the original model to overpredict bioaccumulation is also evident in Figure 2.14 which compares predictions of total PCBs concentrations in lake trout to a long-term dataset provided by DeVault *et al*. (1986 and personal communication). Predictions for several lake trout age classes are plotted, corresponding to the range of average fish age inferred from weight data for the fish composited in these samples. The original model overpredicts total PCBs concentrations in lake trout for all years except for the early 1970s when the highest PCBs concentrations were observed.

The results of the original MICHTOX model simulations were also interrogated in terms of total PCBs mass transport fluxes and inventories for the 1994-1995 period. These are summarized in Table 2.6, with results for Green Bay separated from the main lake. According to the original model, both air-water and water-sediment fluxes dominate the transport of PCBs in Lake Michigan. The negative PCBs flux associated with the Straits of Mackinac export arises from the boundary condition treatment in which higher PCBs concentrations are associated with the reverse-flow component from deeper layers of the water column at this boundary.

2.5.3 Updating Parameterization for Henry's Constants

Henry's constants for PCBs congeners estimated using the Bamford *et al*. (2000) model are significantly higher than those used in the initial MICHTOX parameterization. This is illustrated in Table 2.7 where Henry's constants for the modeled homologs are compared on a monthly basis. These values were calculated from the average Henry's constants for all congeners in each homolog using

Table 2.6. Mass Balance Diagnostics for Total PCBs in the Original MICHTOX Simulation (Year 1994-1995)

	Flux (kg/d)	
Mass Transport Pathway	**Main Lake**	**Green Bay**
Green Bay Export	91	-91
Straits of Mackinac Export	-4	
Chicago River Export	1	
Tributary Loading	128	133
Atmospheric Deposition	137	14
Net Volatilization	1256	391
Volatilization (Gross)	2170	420
Gas Absorption	914	29
Settling	2141	2574
Resuspension	2632	2802
Burial	815	54
Net (Mass In - Mass Out)	-1712	-390
	Inventory (kg)	
Total PCBs Inventory	**Main Lake**	**Green Bay**
Water Column	1630	104
Surficial Sediment	16,500	7530

Table 2.7. Comparison of Original and Revised Henry's Constant (atm m^3/mol) Parameterization

Month	Revised PCB4	Original PCB4	Revised PCB5	Original PCB5
January	1.3E-04	2.5E-05	1.6E-04	2.1E-05
February	1.2E-04	2.5E-05	1.6E-04	2.1E-05
March	1.2E-04	2.5E-05	1.5E-04	2.1E-05
April	1.2E-04	2.5E-05	1.6E-04	2.1E-05
May	1.3E-04	3.7E-05	1.7E-04	3.2E-05
June	1.7E-04	6.2E-05	2.1E-04	5.3E-05
July	2.2E-04	9.9E-05	2.8E-04	8.8E-05
August	2.6E-04	1.4E-04	3.2E-04	1.2E-04
September	2.4E-04	1.2E-04	3.0E-04	1.1E-04
October	1.9E-04	7.4E-05	2.4E-04	6.4E-05
November	1.6E-04	6.2E-05	2.0E-04	5.3E-05
December	1.4E-04	3.7E-05	1.8E-04	3.2E-05
Annual Average	1.7E-04	6.1E-05	2.1E-4	5.2E-05

the mean monthly temperature. The Bamford Henry's constants are two to seven times higher than the original values which were based on data from Burkhard (1984). Interestingly, the model based upon Bamford's measurements predicted that the higher molecular weight congeners had generally higher Henry's constants. This was a consequence of the number of ortho-chlorine substitutions, which the model correlated to volatility, increasing with molecular weight (i.e., homolog number). Previously, higher chlorinated PCBs had generally been assumed to be less volatile (Brunner *et al*., 1990; Dunnivant *et al*., 1992).

2.5.4 Updating the Chemical Volatilization Rate Formulations

The total PCBs volatilization rates calculated using the Wanninkhoff (1992) and Schwarzenbach *et al*. (1993) formulations were substantially higher than the rates computed in the original MICHTOX model. Monthly rates of PCBs homolog volatilization, calculated using the original and revised MICHTOX formulations, are compared in Table 2.8. The revised volatilization rates are two to three times higher than those computed in the original model. The revised volatilization mass transfer rate calculations were confirmed by reproducing the congener-specific rates presented in Totten *et al*. (2001). The original model computed volatilization rates using the formulations of O'Connor (1983) and Liss (1973).

In terms of PCBs transport and fate, the implications of higher Henry's constants and volatilization rates is that PCBs equilibrium will be shifted significantly towards the atmospheric vapor phase, and this shift will occur more rapidly than previously predicted.

2.5.5 Long-Term Hindcast/Forecast Simulations

The first simulations conducted with the revised MICHTOX model were long-term simulations from a zero (i.e., "clean") initial condition in 1940. These were conducted for each of the long-term forcing function scenarios: A, B, and C. The results of these simulations were compared to LMMBP and long-term PCBs concentration data, with the goals of confirming model predictions and determining which long-term loading scenario best simulated the data. Predictions for Scenario A, in which the PCBs forcing functions were assumed to peak in 1970-1972, are plotted and compared to data in Figures 2.15 to 2.19. Predictions in the main Lake Michigan segments are compared to available water column measurements (including those from the LMMBP) in Figure 2.15. Clearly, the model predictions of total PCBs concentration in the water column are low for this scenario. For reference, the Scenario A predictions in the southern Lake Michigan segments (Segments 1 and 8) are plotted together with the original model long-term predictions in Figure 2.16. Predicted surficial sediment total PCBs concentrations are also very low in comparison to the data as shown in

Table 2.8. Monthly PCBs Volatilization Rates (m/d) Calculated by Original and Revised MICHTOX Formulations

Month	Original PCB4 Rate	Revised PCB4 Rate	Original PCB5 Rate	Revised PCB5 Rate
January	0.44	1.72	0.37	1.83
February	0.42	1.63	0.36	1.74
March	0.41	1.59	0.35	1.71
April	0.39	1.52	0.33	1.63
May	0.45	1.26	0.39	1.34
June	0.37	0.75	0.33	0.77
July	0.37	0.55	0.34	0.56
August	0.61	0.74	0.55	0.74
September	1.05	1.27	0.93	1.29
October	0.98	1.72	0.85	1.78
November	0.98	0.95	0.85	2.02
December	0.60	1.72	0.52	1.81
Annual Average	0.59	1.29	0.51	1.43

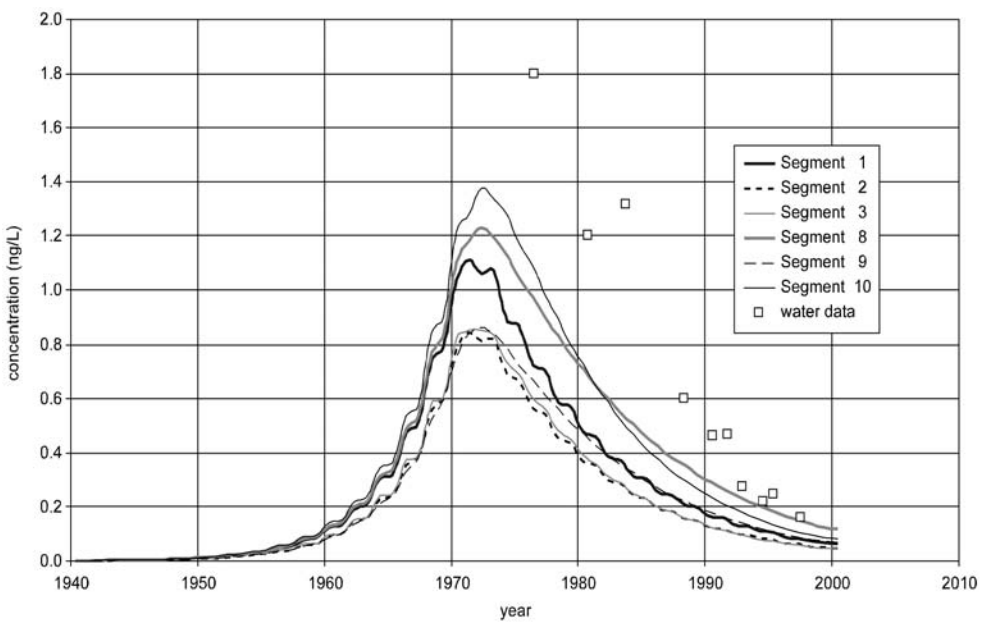

Figure 2.15. Long-term Scenario A predictions of main lake total PCBs concentrations.

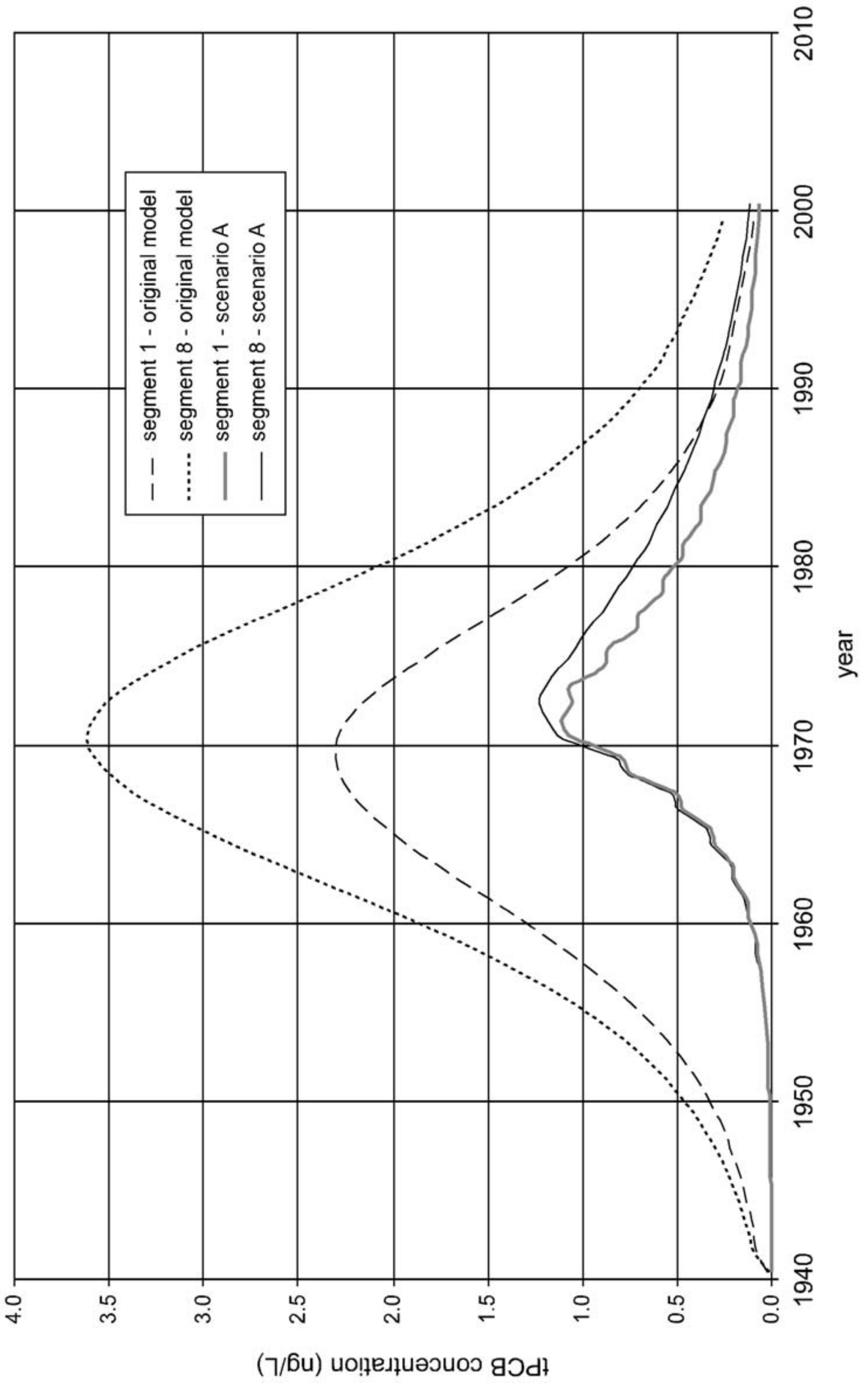

Figure 2.16. MICHTOX southern Lake Michigan total PCBs predictions. Comparison of long-term Scenario A to original model predictions.

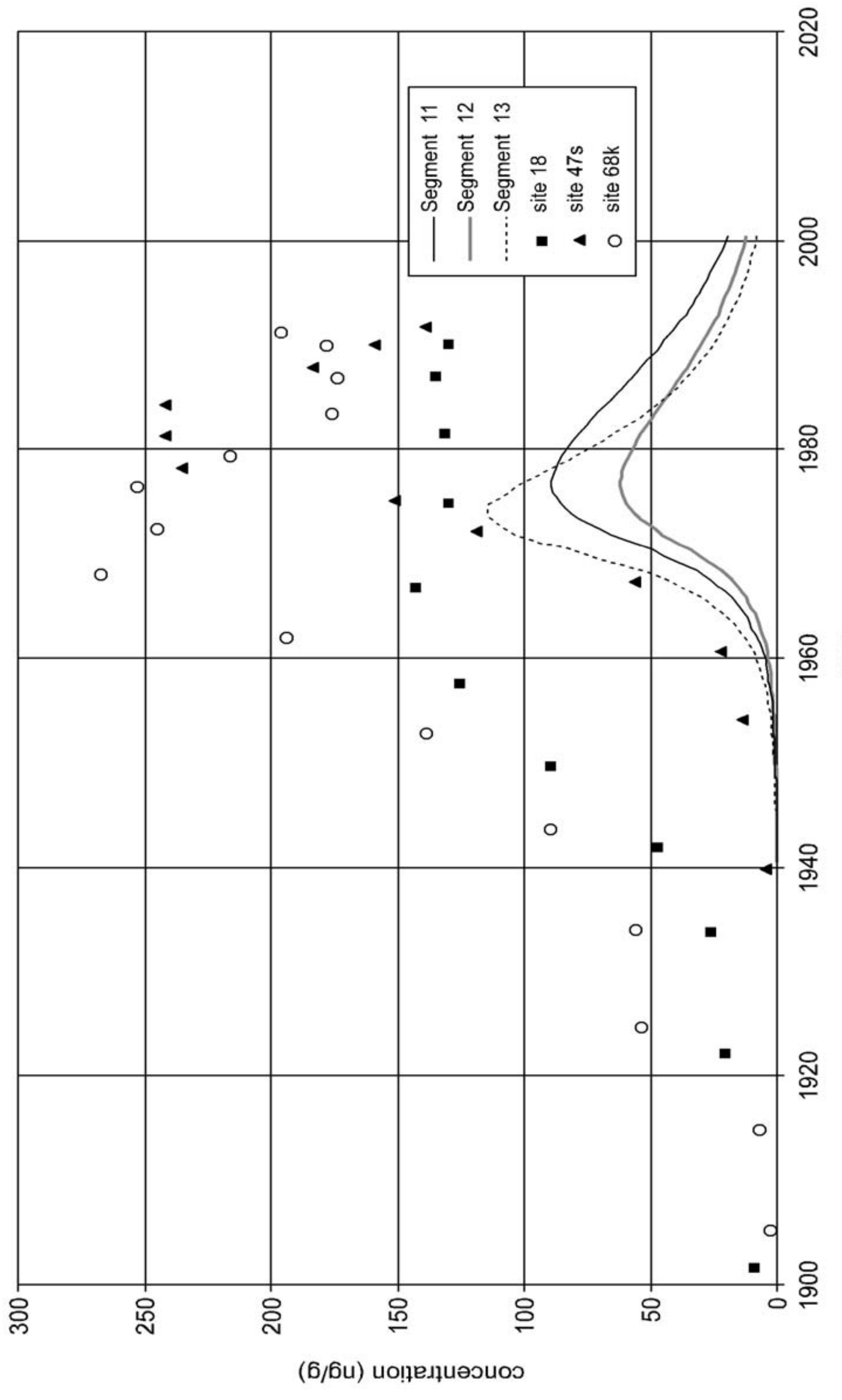

Figure 2.17. Comparison of long-term Scenario A predictions to main lake sediment total PCBs concentrations (sediment cores collected in 1991-1992).

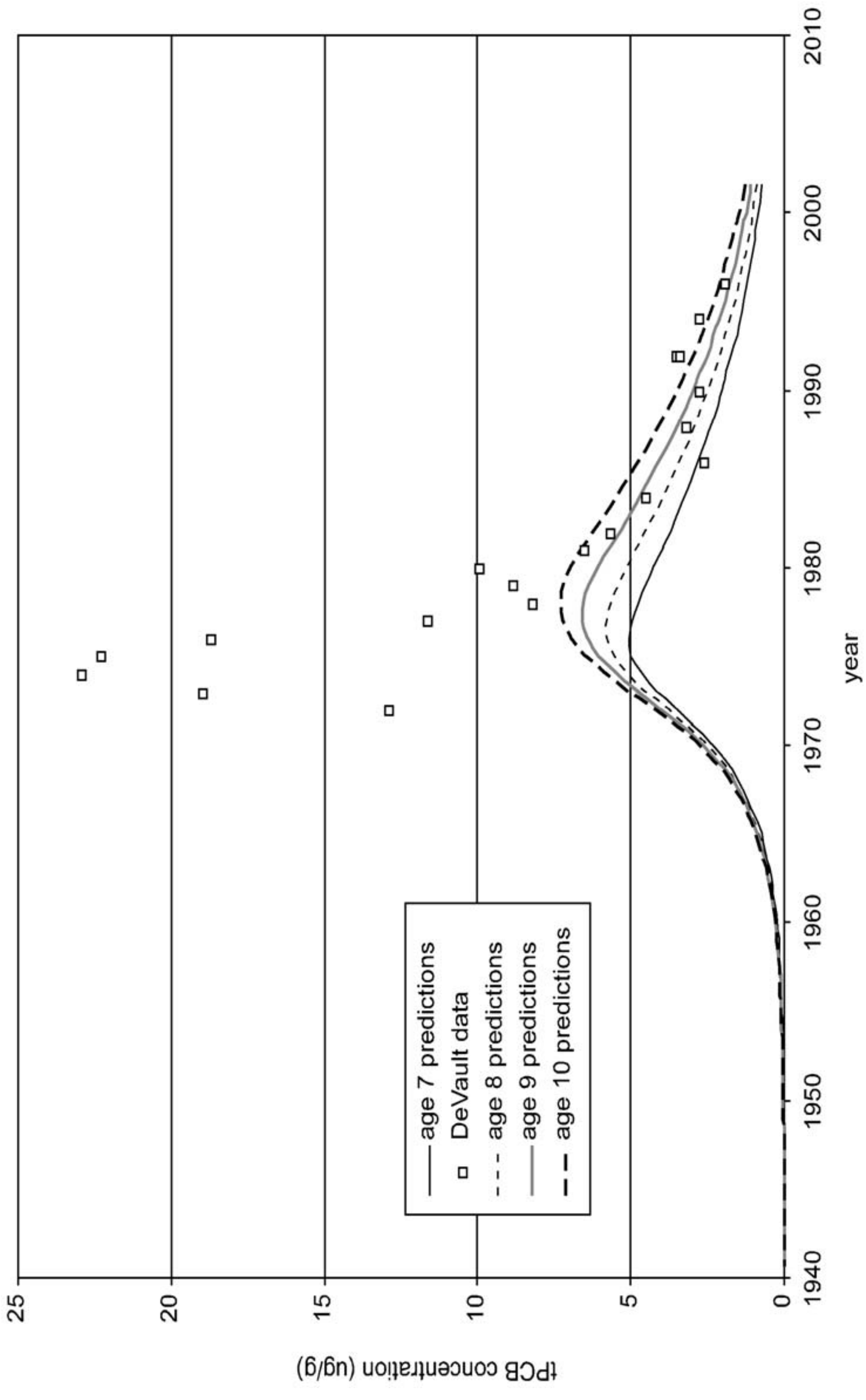

Figure 2.18. Comparison of long-term Scenario A predictions to DeVault *et al*. (1986) lake trout data.

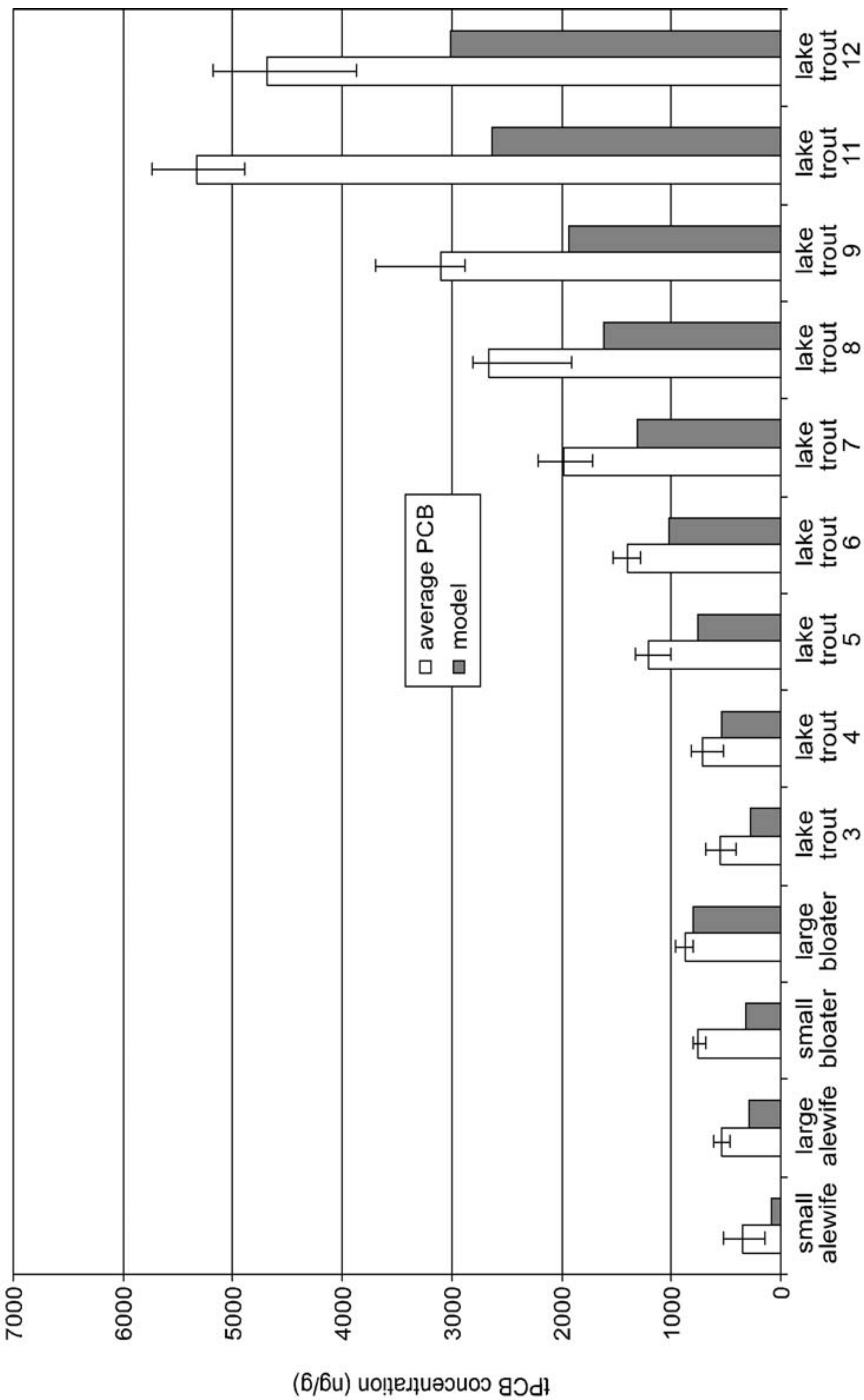

Figure 2.19. Comparison of MICHTOX Scenario A total PCBs concentrations to Sheboygan Reef data.

Figure 2.17. The same tendency of Scenario A to underpredict total PCBs concentrations occurs with the fish data, both DeVault's long-term data (Figure 2.18) and the size- and age-class specific data from the LMMBP (Figure 2.19).

Predictions for Scenario B, in which the PCBs forcing functions were assumed to peak in 1961-1963, are plotted and compared to data in Figures 2.20-2.29. Predictions in the main Lake Michigan segments are compared to available water column measurements (including those from the LMMBP) in Figure 2.20. Although still somewhat low, Scenario B predictions are definitely an improvement over Scenario A. Scenario B water column predictions are also compared to the original MICHTOX model predictions in Figure 2.21. Figure 2.22 compares the deepwater (hypolimnetic) predicted dissolved total PCBs concentrations to segment-average data for the eight LMMBP cruises. The model accurately predicts both the trend of decreasing dissolved total PCBs concentrations moving from south to north in the lake, as well as the build-up of deepwater dissolved total PCBs concentrations during the stratified period of each year. This agreement is encouraging because dissolved-phase deepwater concentrations were used as PCBs exposure concentrations for the bioaccumulation model.

Predicted surficial sediment total PCBs concentrations for Scenario B are compared to sediment core data in Figure 2.23. The comparison of model predictions to average surficial sediment concentrations based on LMMBP sediment core samples (Figure 2.24) is somewhat more informative. Surficial sediment total PCBs concentrations in southern and central Lake Michigan and mid-Green Bay are about 60% low in comparison to the data, while predicted sediment concentrations are much closer to average concentrations measured in other sediment segments.

Scenario B predictions of total PCBs concentrations in fish are compared to DeVault's (DeVault, 1986; DeVault, personal communication) long-term data (Figure 2.25) and the size- and age-class specific data from the LMMBP for Sheboygan Reef (Figure 2.26). In general, this simulation compares well with both the long-term and LMMBP data, although aspects of both simulations deserve comment. The Scenario B lake trout predictions agree well with long-term data after the mid-1970s; however, they locate the peak total PCBs concentrations about five years earlier than observed by DeVault. The lake trout total PCBs predictions are also 20-30% lower than the data for most of the Sheboygan Reef age class data. In general, however, the Scenario B simulations offer a better prediction of the total PCBs data than the original MICHTOX model simulation.

The results of the Scenario B MICHTOX model simulations were also interrogated in terms of total PCBs mass transport fluxes and inventories for the 1994-1995 period. These are presented in Table 2.9. Comparison of these results to the mass balance diagnostics from the original model (Table 2.6) demonstrate how the transport and fate predictions for PCBs have changed as a result of updating the Henry's constant parameterization, revising the volatilization rate formulations, and making use of the LMMBP estimates to develop long-term PCBs forcing functions. Most notably, the total PCBs inventories are depleted by 40-70% in the Scenario B simulation (in comparison to the original long-term model simulation) due to the increased chemical volatility.

Enhanced volatility of total PCBs completely offsets the enhanced absorption resulting from higher vapor concentrations. Scenario B mass balance diagnostics also demonstrate that air-water fluxes now clearly predominate the transport pathways for PCBs in Lake Michigan.

Predictions for Scenario C, in which the PCBs forcing functions were assumed to peak over a longer duration, from 1961-1972, are plotted and compared to data in Figures 2.27-2.31. Although Scenario C forcing functions are substantially different, the predictions are qualitatively similar to those for Scenario B, at least for the period during which data are available.

In general, the Scenario B long-term simulations tend to agree most favorably with the available PCBs data. The model predictions for this scenario are probably at least as accurate as the forcing functions themselves; this was judged to be an adequate level of model confirmation for this assessment. Further refinement of forcing functions and model parameters could improve the agreement between data and predictions; however this was not possible given the time and resource constraints of this project.

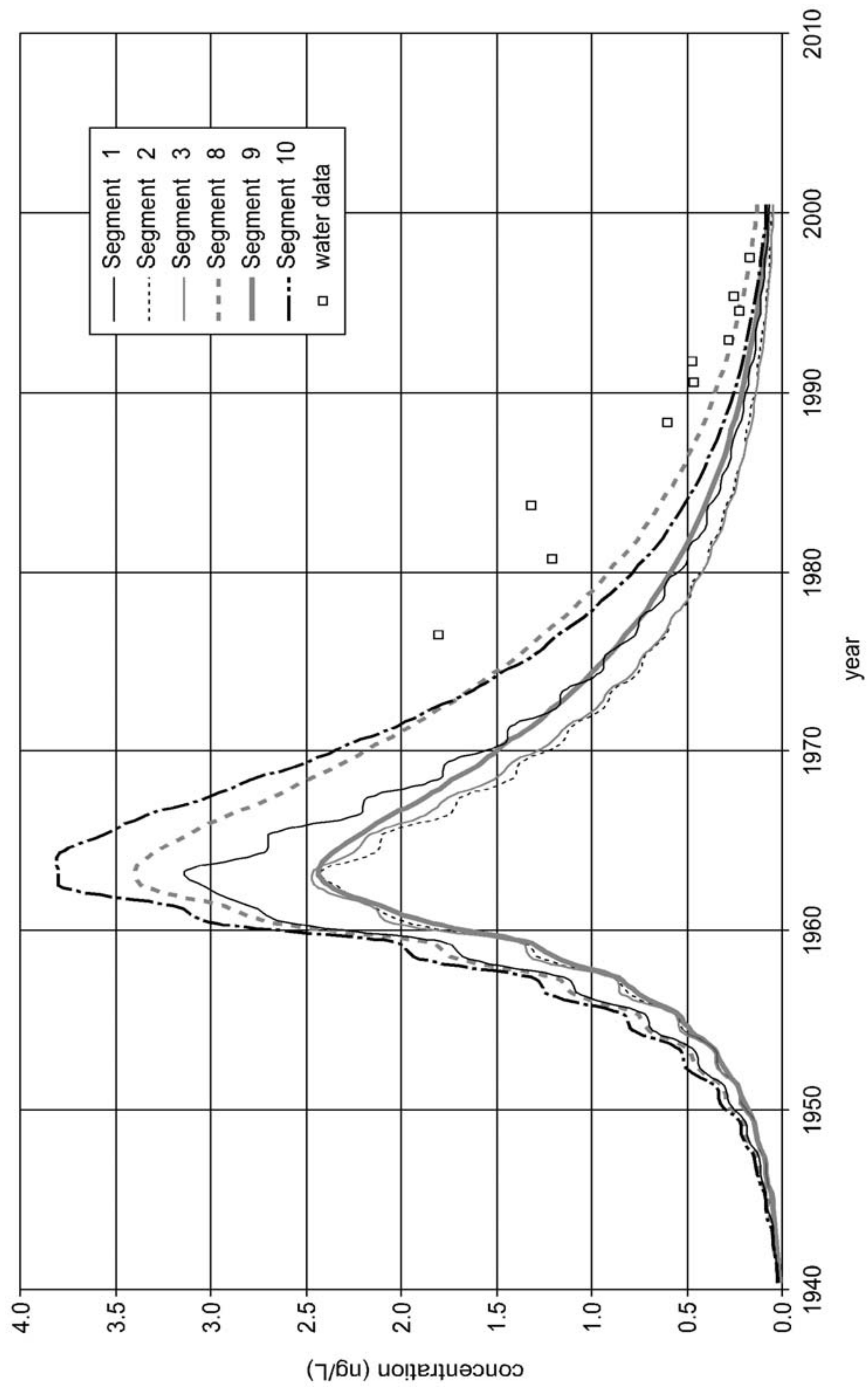

Figure 2.20. Long-term Scenario B predictions of main lake total PCBs concentrations.

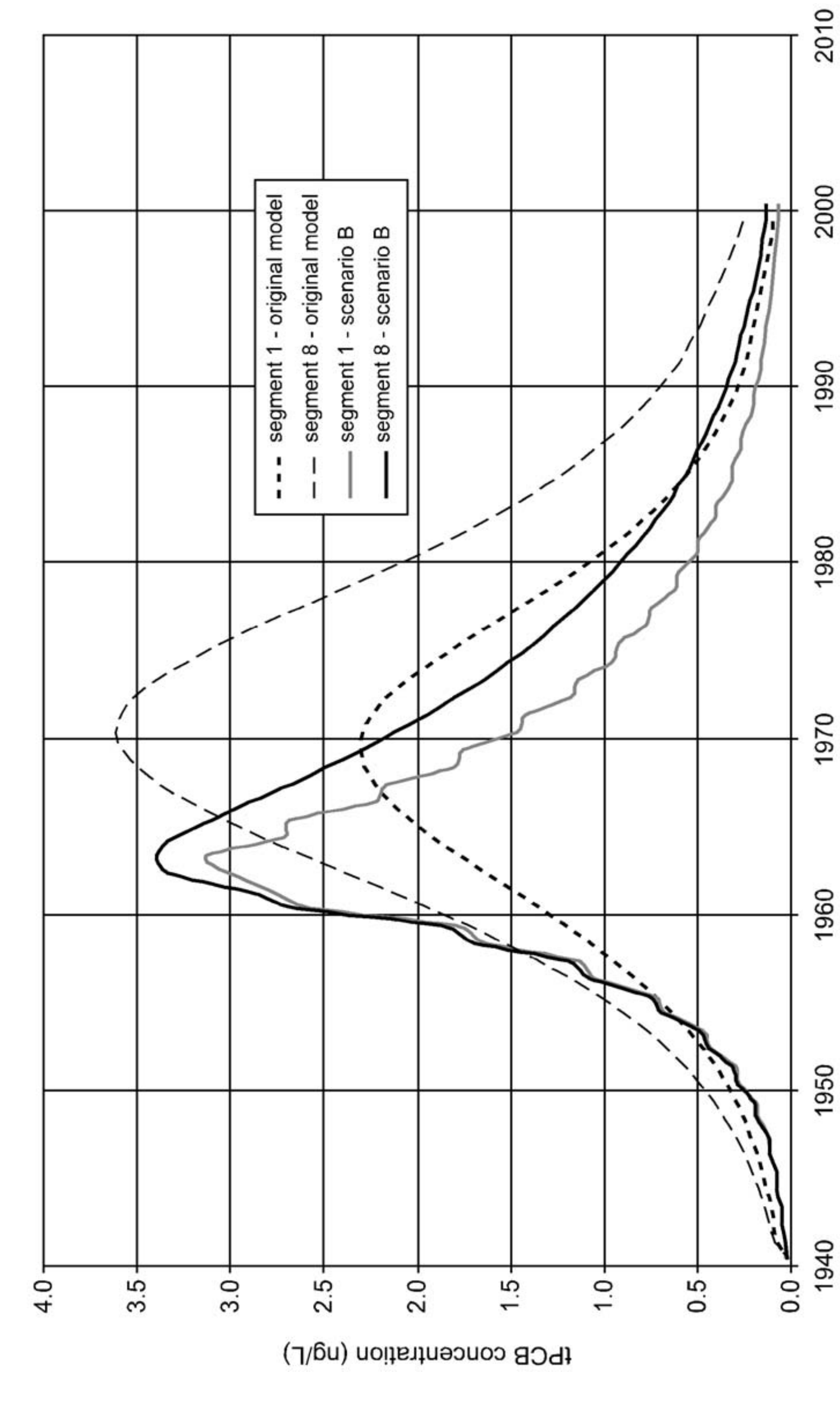

Figure 2.21. MICHTOX southern Lake Michigan total PCBs predictions. Comparison of long-term Scenario B to original model predictions.

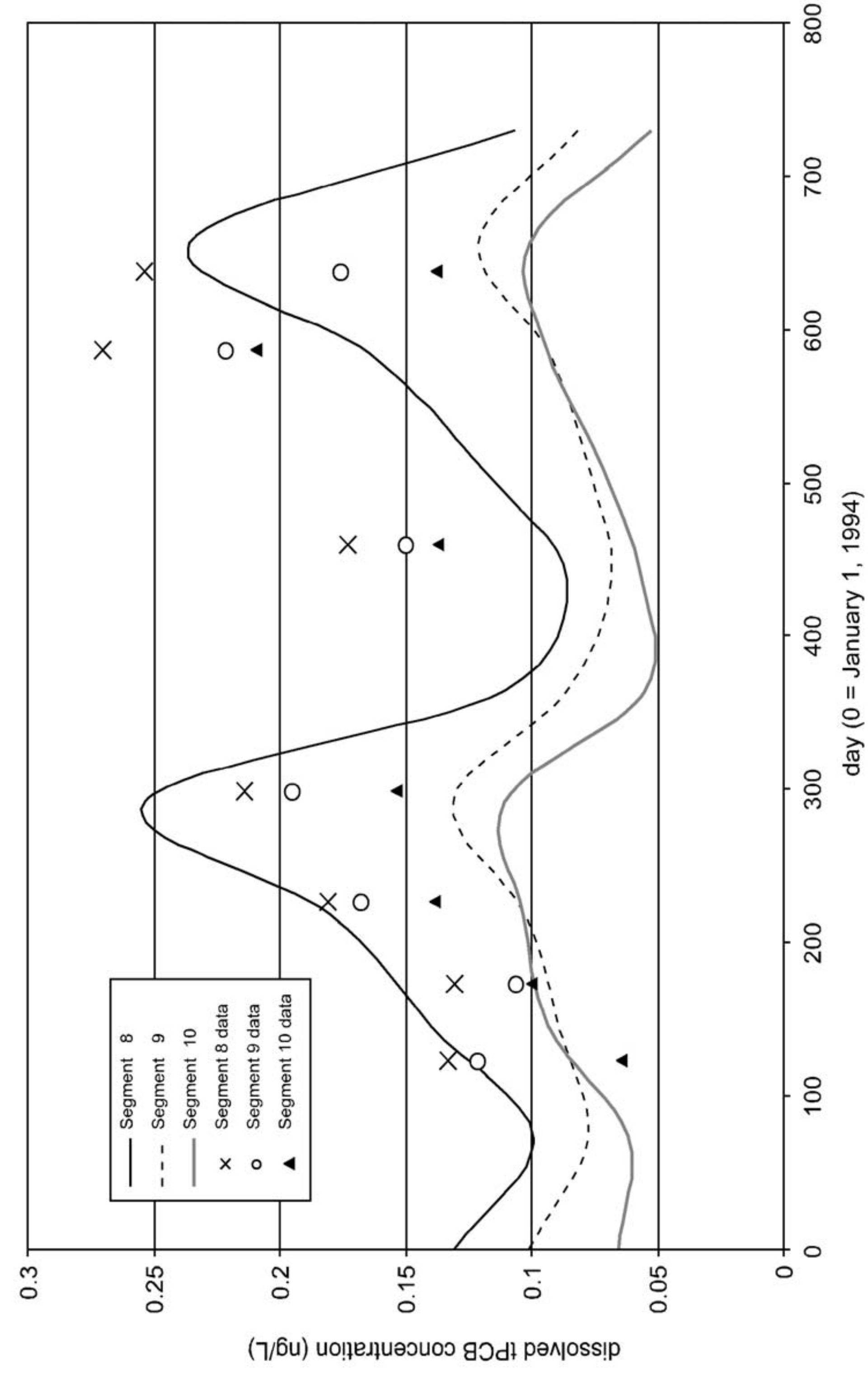

Figure 2.22. Comparison of long-term Scenario B predictions to the LMMBP deepwater dissolved total PCBs concentrations.

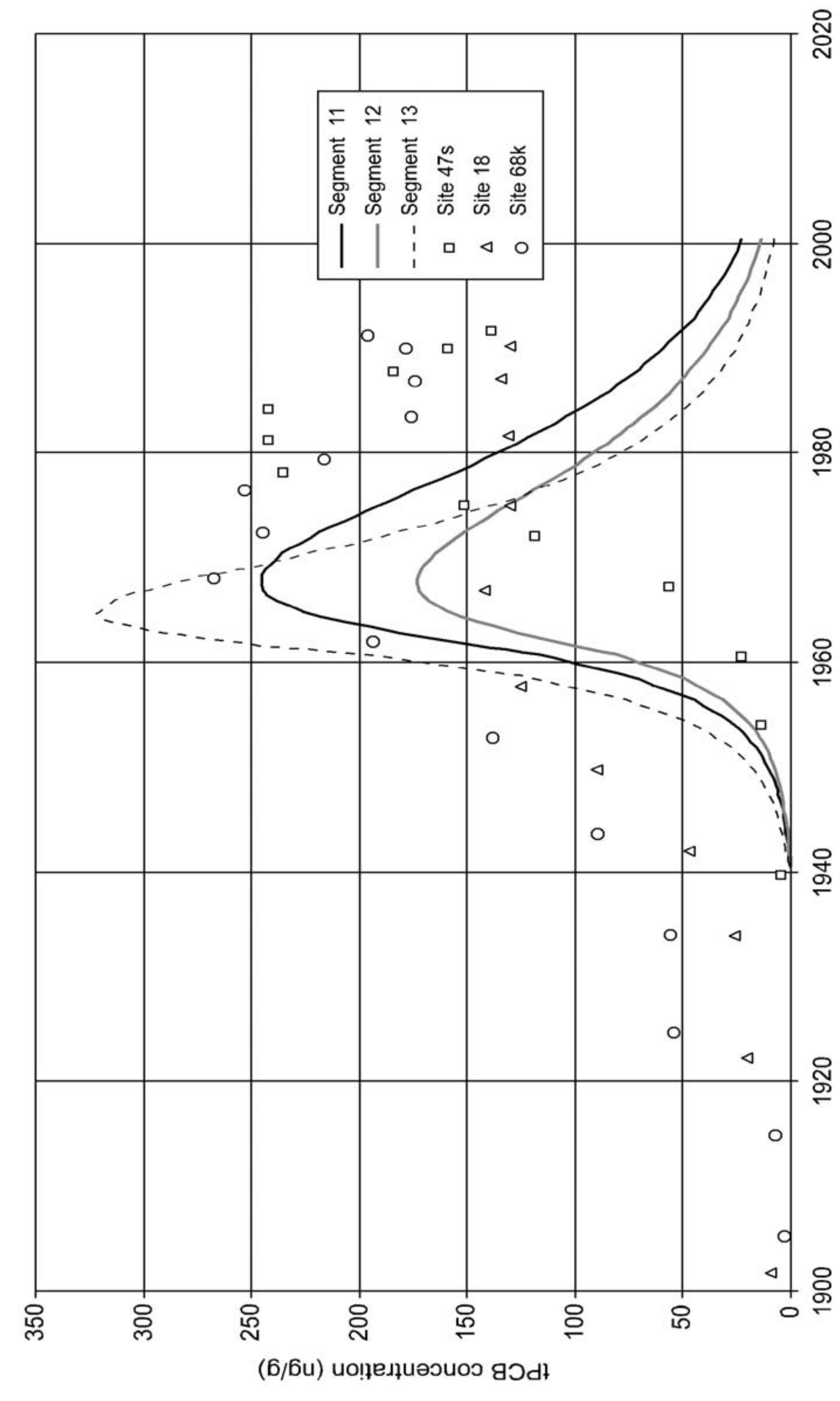

Figure 2.23. Comparison of Scenario B predictions to main lake sediment total PCBs concentrations (sediment cores collected in 1991-1992).

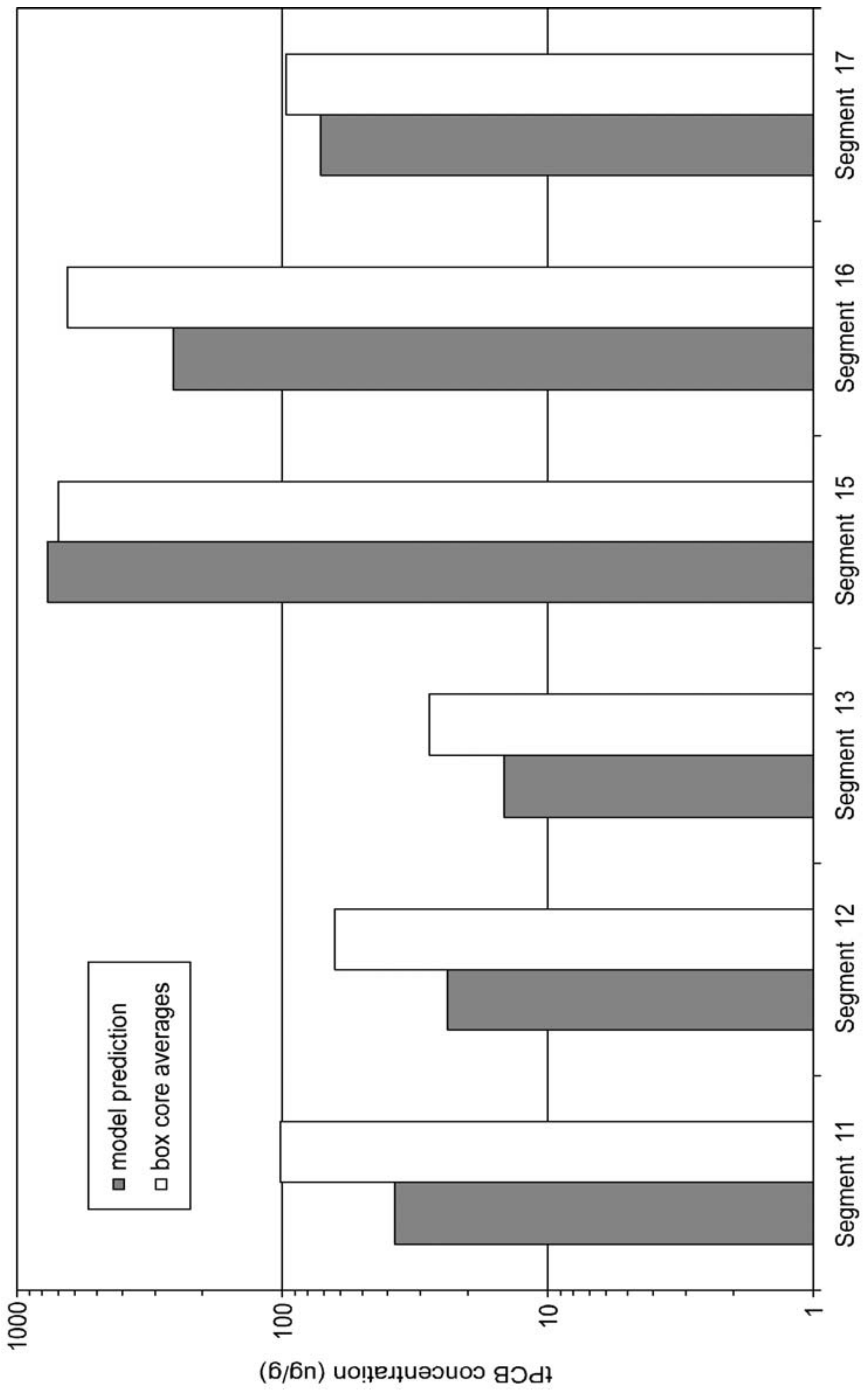

Figure 2.24. Comparison of long-term Scenario B predictions to average total PCBs sediment concentrations (LMMBP and GBMBP box core samples).

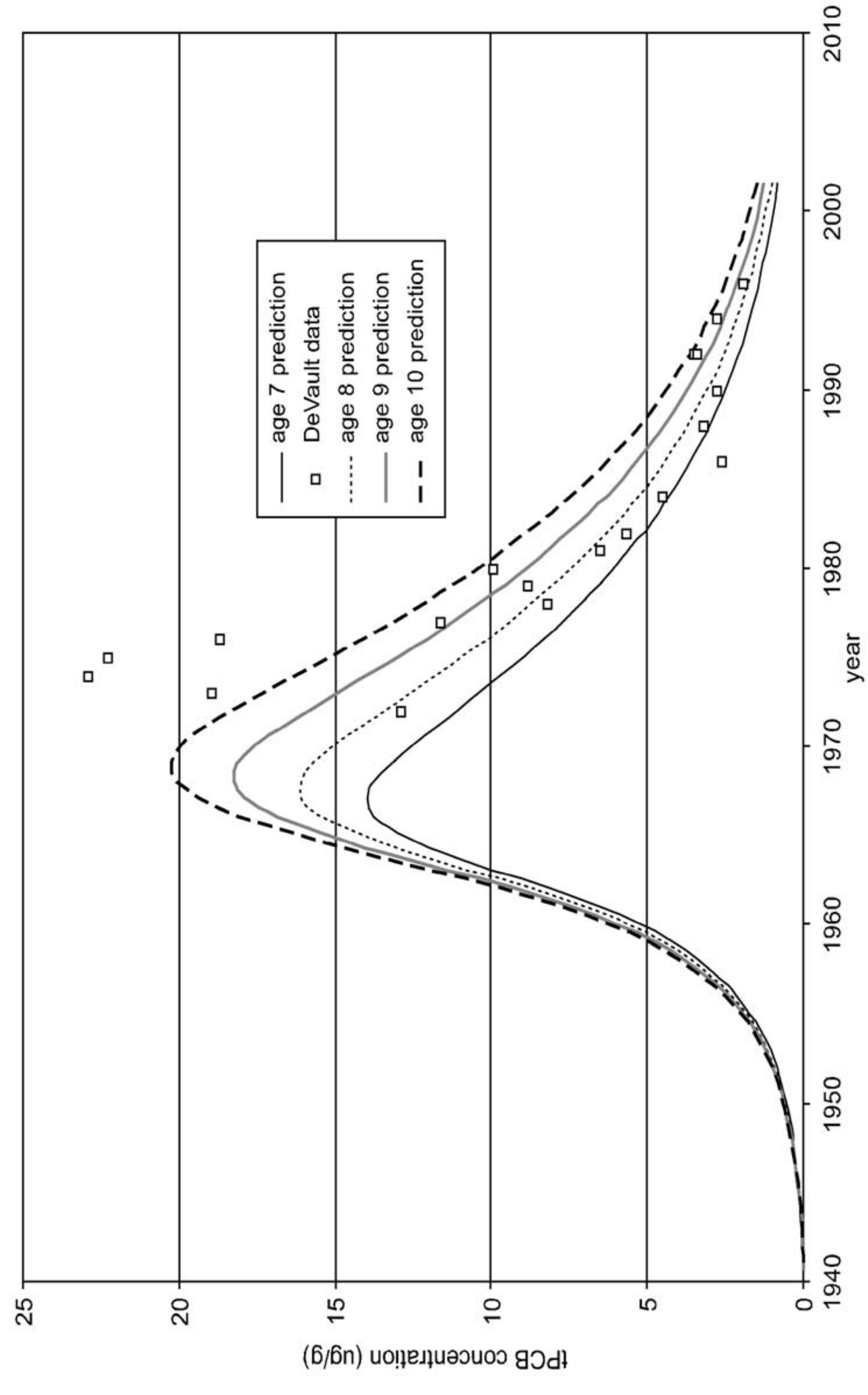

Figure 2.25. Comparison of long-term Scenario B predictions to DeVault *et al*. (1986) lake trout data.

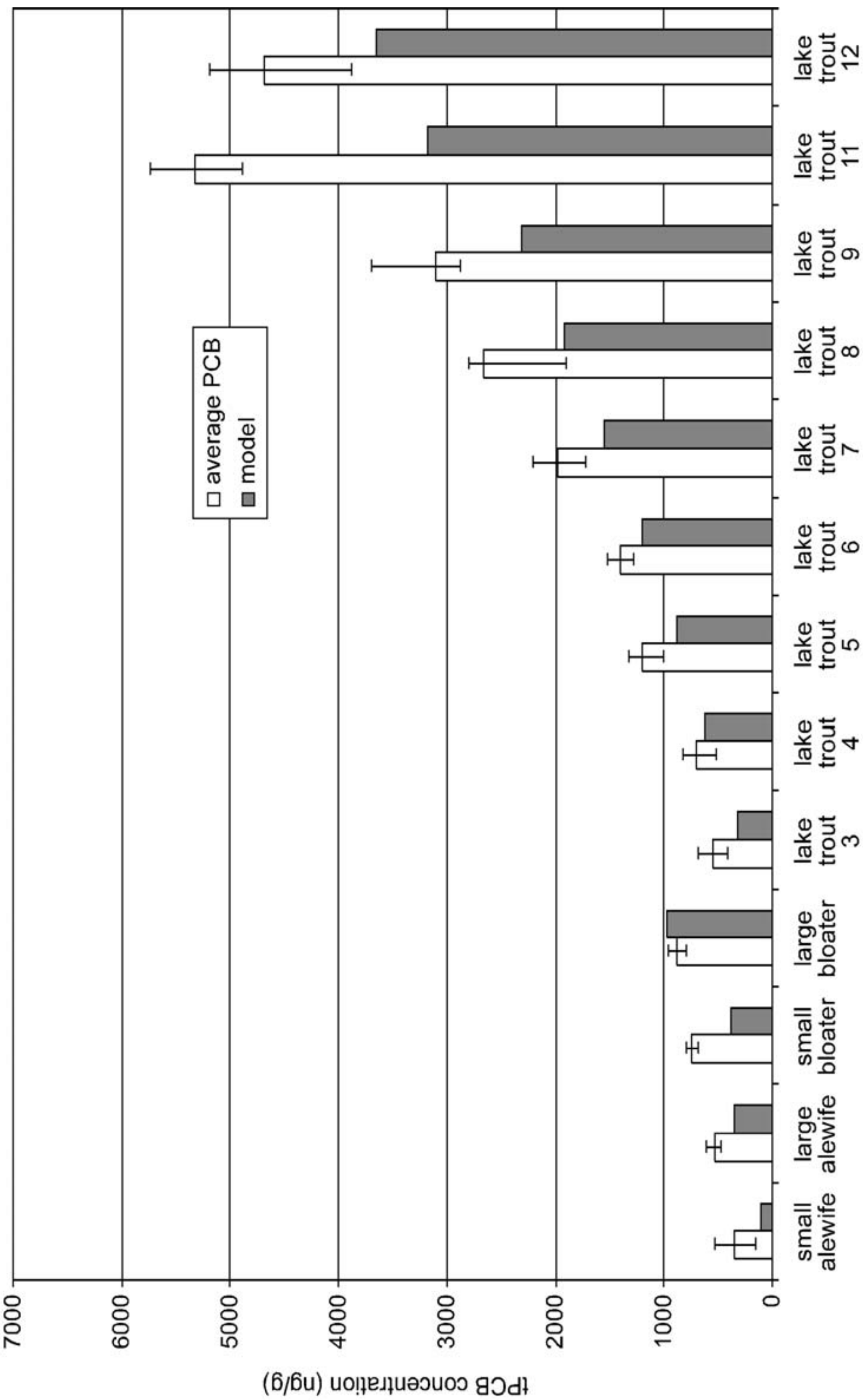

Figure 2.26. Comparison of long-term Scenario B total PCBs concentrations to Sheboygan Reef fish data.

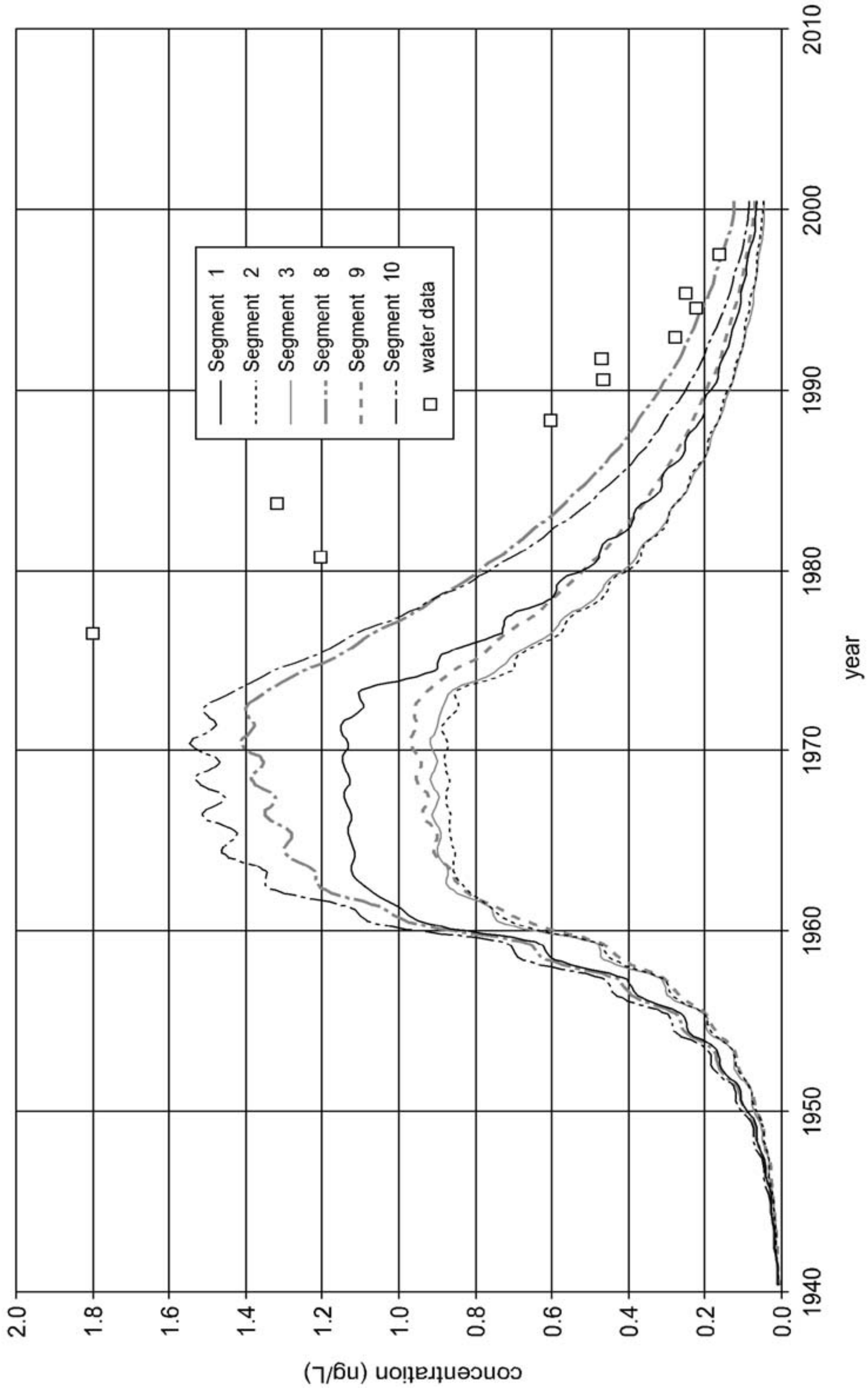

Figure 2.27. Long-term Scenario C predictions of main lake total PCBs concentrations.

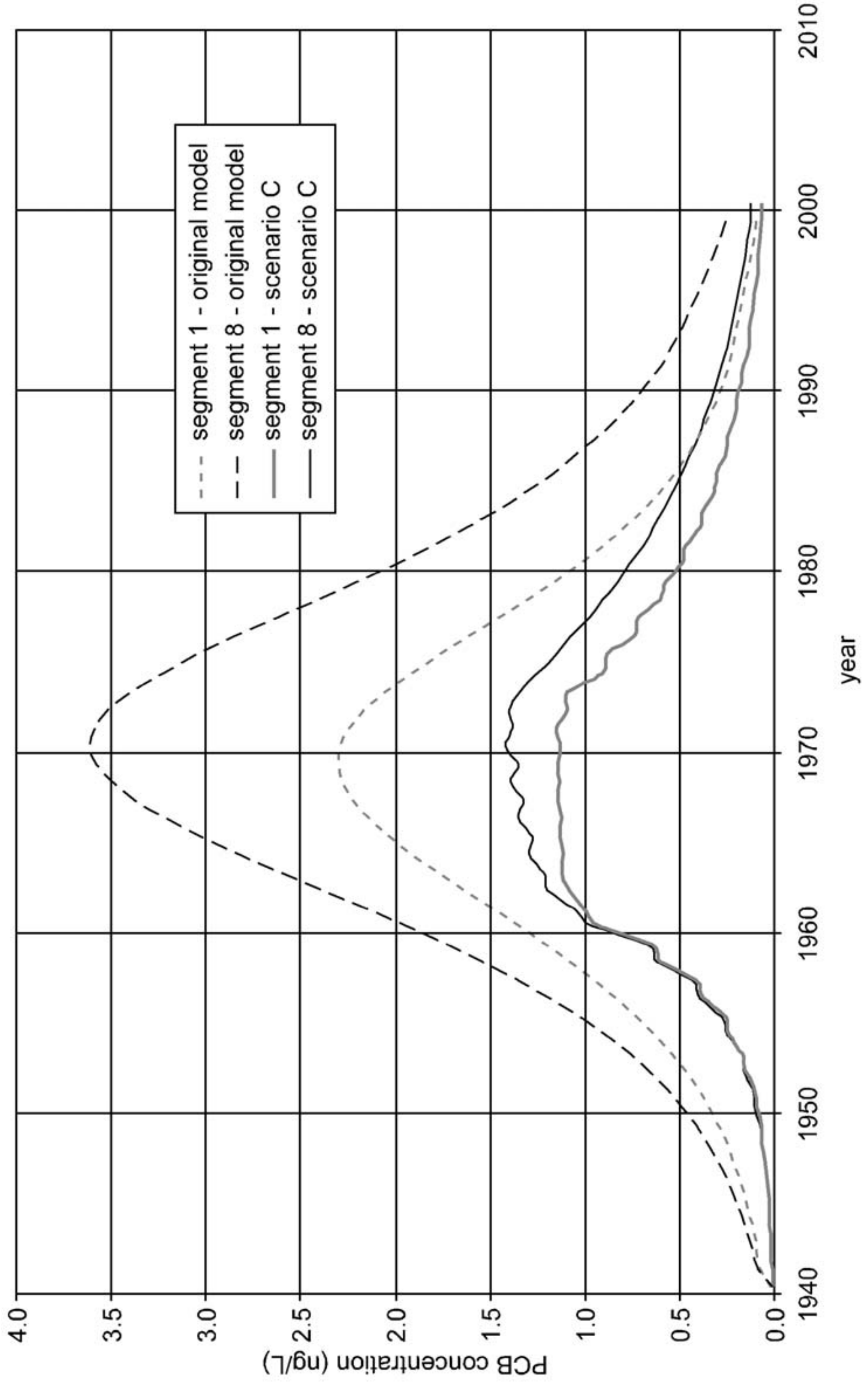

Figure 2.28. MICHTOX southern Lake Michigan total PCBs predictions. Comparison of long-term Scenario C to original model predictions.

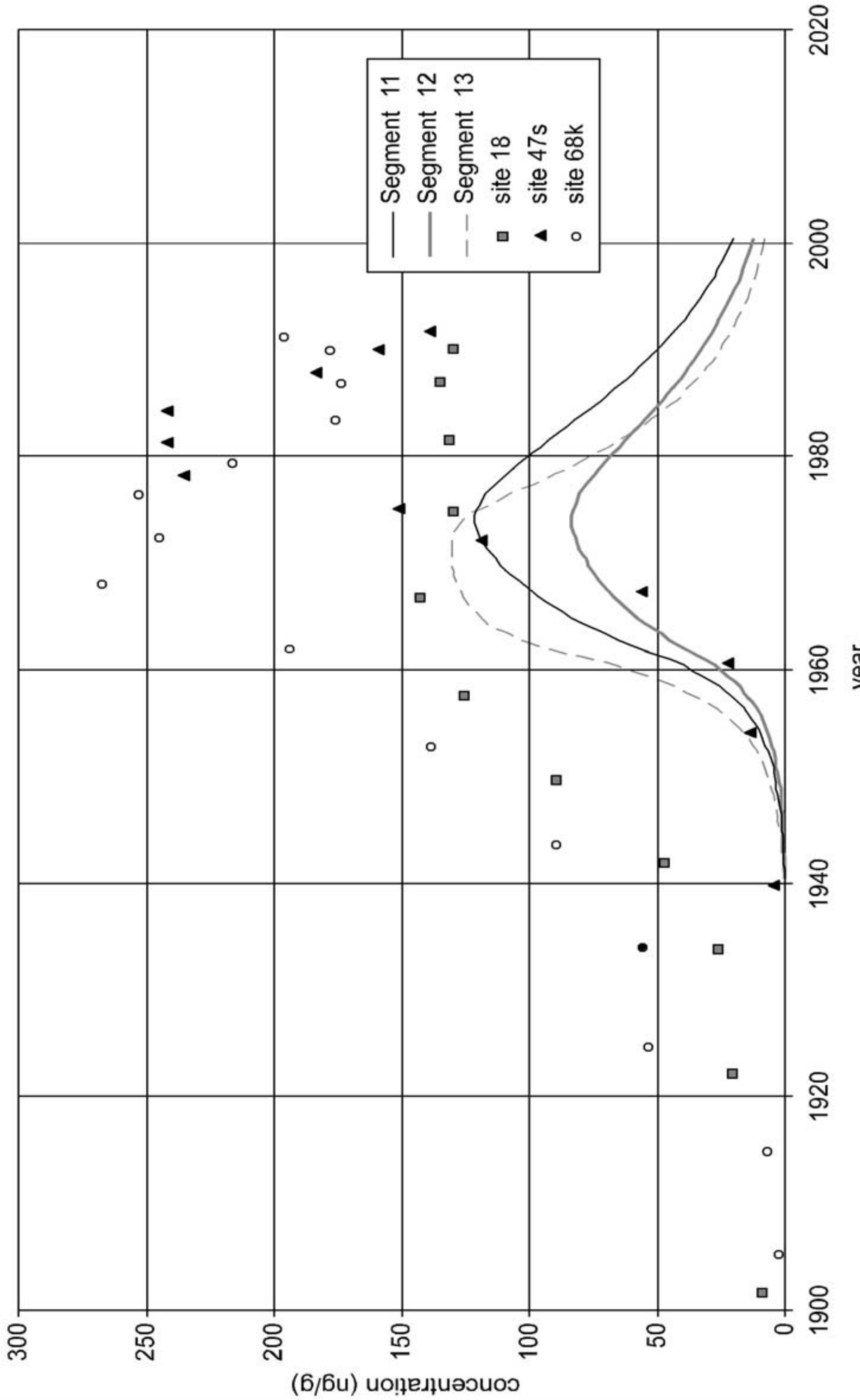

Figure 2.29. Comparison of Scenario C predictions to main lake sediment total PCBs concentrations (sediment cores collected in 1991-1992).

Table 2.9. Mass Balance Diagnostics for Total PCBs in MICHTOX Scenario B Simulation (Year 1994-1995)

	Flux (kg/d)	
Mass Transport Pathway	**Main Lake**	**Green Bay**
Green Bay Export	38	-38
Straits of Mackinac Export	0	
Chicago River Export	0	
Tributary Loading	126	220
Atmospheric Deposition	216	15
Net Volatilization	758	432
Volatilization (Gross)	3000	502
Gas Absorption	2243	70
Settling	948	1641
Resuspension	1152	1811
Burial	349	28
Net (Mass In - Mass Out)	-726	-262
	Inventory (kg)	
Total PCBs Inventory	**Main Lake**	**Green Bay**
Water Column	690	57
Surficial Sediment	7070	4370

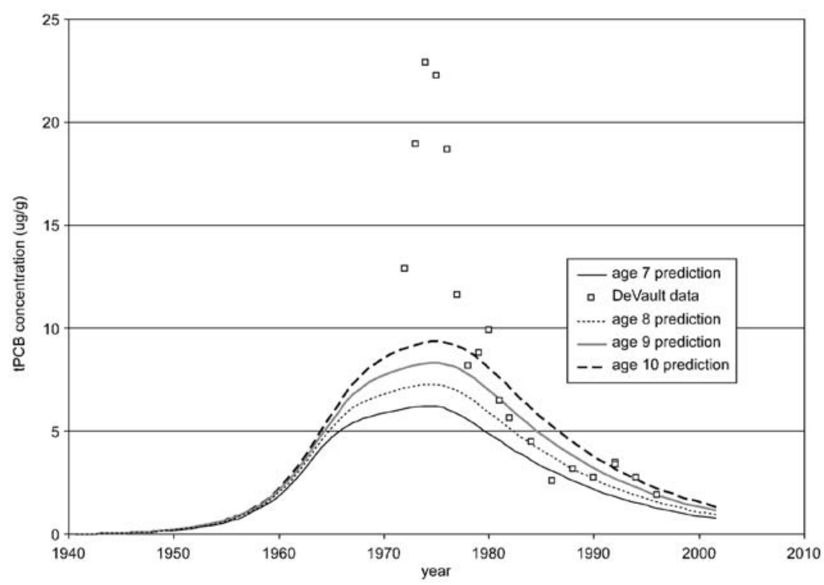

Figure 2.30. Comparison of long-term Scenario C predictions to DeVault *et al*. (1986) lake trout data.

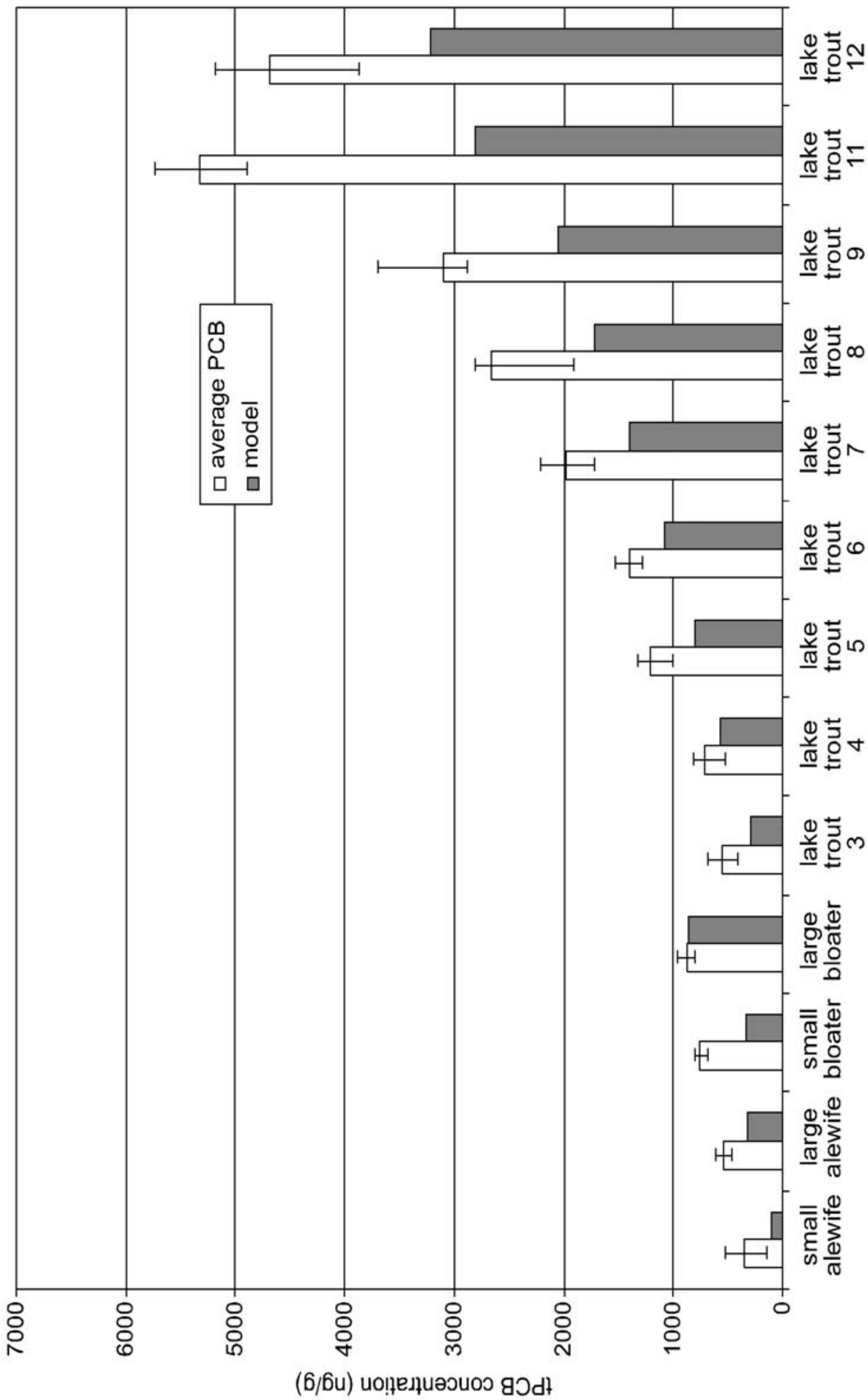

Figure 2.31. Comparison of MICHTOX Scenario C total PCBs concentrations to Sheboygan Reef fish data.

Although it is tempting to conclude from the model confirmation, that long-term forcing functions such as Scenario B are accurate estimates of past PCBs inputs to Lake Michigan, it must be cautioned that these estimates are highly speculative. For example, according to the Scenario B estimates, the cumulative tributary loading of PCBs to Lake Michigan through 2002 is 41,000 kilograms. It is not clear how this estimate could be reconciled with Swackhamer and Armstrong's (1988) estimate that 500,000 kg of PCBs were released to Lake Michigan from Waukegan Harbor alone. Clearly, the timing and magnitude of a PCBs input, such as Waukegan Harbor, would have a profound impact on model simulations. It is very difficult to make reliable estimates of past forcing functions for PCBs that are both consistent with, and constrained by, the available data.

2.5.6 Toxic Chemical Management Forecasts

The revised MICHTOX model was next applied to forecast total PCBs concentrations in lake trout for a number of scenarios in which the future PCBs forcing functions were changed from their 1994-1995 estimated values. These changes were intended to represent alternative strategies for managing PCBs in Lake Michigan, and MICHTOX was used to forecast the effectiveness of these alternatives in terms of reducing lake trout total PCBs concentrations. The forecast simulations commenced in 1994 using LMMBP average total PCBs concentrations to define initial conditions in water, sediment, and fish. Forcing functions were changed starting in year 2002 of the simulations, which was treated as the effective date of the scenario-specific control actions. The predictions for total PCBs concentrations in age seven lake trout in the southern lake segment are displayed in Figure 2.32. With the exception of the No-Action scenario, all forecast predictions are the same until simulation year 2002, at which point predictions diverge due to changes in the forcing functions. None of the forecasts reach steady-state (i.e., constant total PCBs concentrations) within the 12 years simulated following the control actions. These predictions are also presented in Table 2.10 in terms of total PCBs concentrations five and ten years after the change in forcing functions.

The No-Change and Elimination scenarios bracket the range of possibilities, in terms of total PCBs concentrations in lake trout, that can be expected as a result of managing loadings and forcing functions. The No-Action forecast predicts that total PCBs concentrations in lake trout will decline by 50% in 10 years, if loadings and vapor concentrations continue over this period at their 1994-1995 levels. This decline occurs because the inventory of total PCBs in the lake sediments is being slowly depleted by volatilization and burial processes, and this depletion results in declining exposure concentrations in both the water column and the surficial sediment. The Elimination forecast predicts that total PCBs concentrations in lake trout will decline by 75% in 10 years if loadings and vapor concentrations are eliminated in 2002. According to these predictions, the maximum achievable reduction in future lake trout total PCBs concentrations over this 10-year period is from 0.82 to 0.38 µg/g, or 55%. This reduction would require the cessation of all PCBs inputs to Lake Michigan.

The Fifty-Percent Forcing Function Reduction and the Fifty-Percent Loading Reduction scenarios explore the effectiveness of incremental toxic chemical management alternatives. As expected, the Fifty-Percent Forcing Function Reduction scenario is forecast to be half as effective as Elimination in terms of predicted total PCBs concentrations in lake trout after 10 years. The forecast total PCBs concentration is 0.60 µg/g after 10 years, a 60% reduction from the predicted concentration in 2002. The Fifty-Percent Loading Reduction scenario demonstrates how the effectiveness of toxic chemical management is diminished if atmospheric vapor concentrations are not brought under control. For this scenario, tributary and atmospheric deposition loadings are reduced 50%, but vapor concentrations are held at 1994-1995 values. In this case, the forecast total PCBs concentration is 0.77 µg/g after 10 years, only a 50% reduction from the predicted concentration in 2002, and only six percent lower than the 10-year concentration forecast for the No-Change scenario.

The No-Action scenario differs from the others. It assumes that atmospheric vapor concentrations will continue to decline in the future according to the rate of decline observed over the past 25 years. As noted previously, there is no scientific consensus as to

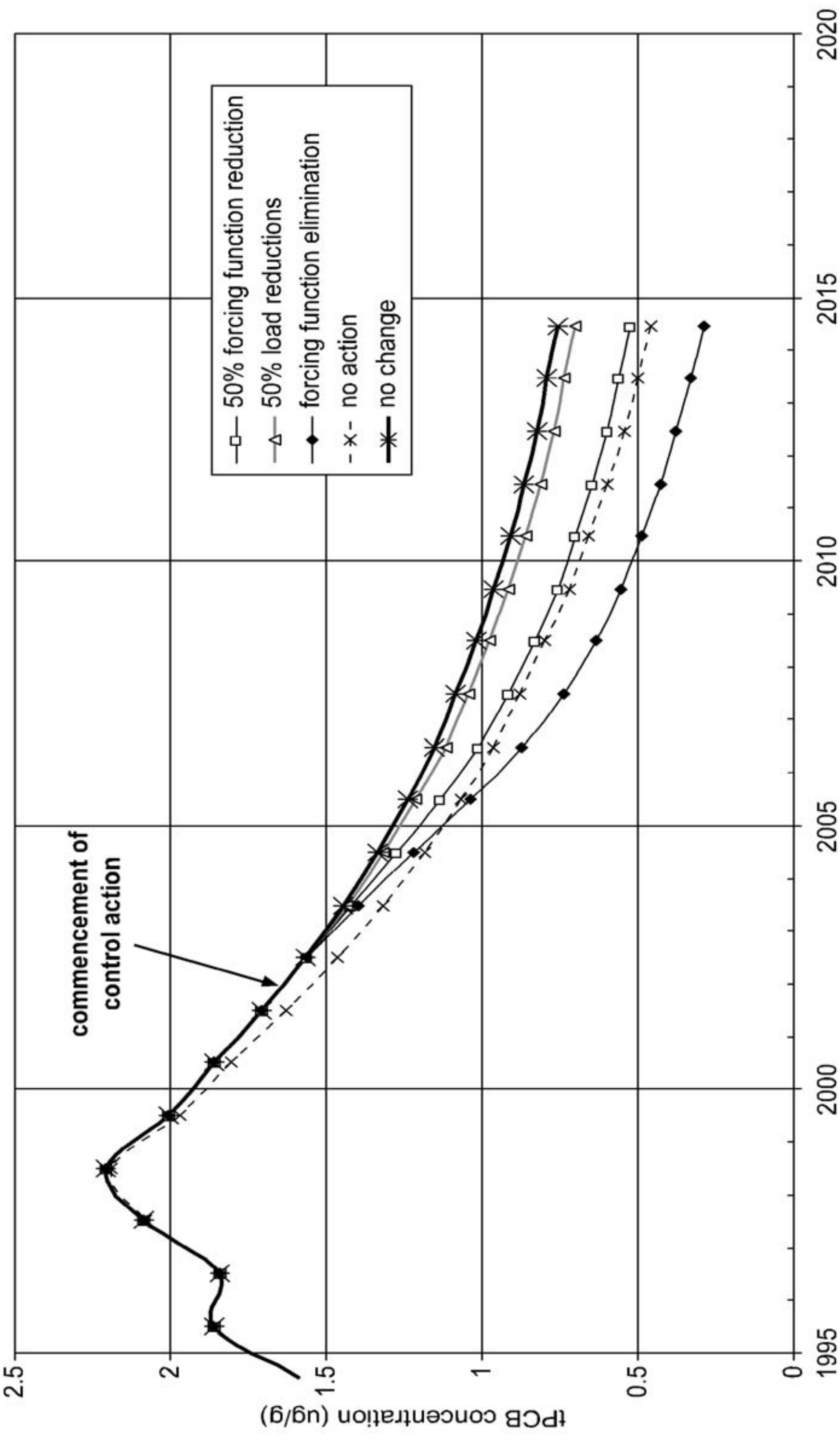

Figure 2.32. Toxic chemical management alternatives. Comparison of forecast simulation for age seven lake trout in southern Lake Michigan.

Table 2.10. MICHTOX Predictions of Total PCBs Concentrations (µg/g) in Lake Trout for Toxic Chemical Management Alternatives

	Years After Action		
Simulated Control Action	0	5	10
No-Change	1.57	1.09	0.82
No-Action	1.46	0.88	0.55
Fifty-Percent Forcing Function Reduction	1.56	0.91	0.60
Fifty-Percent Loading Reduction	1.57	1.04	0.77
Forcing Function Elimination	1.56	0.74	0.38

whether this is a realistic expectation. For this scenario, the forecast total PCBs concentration is 0.55 µg/g after 10 years, a 60% reduction from the predicted concentration in 2002. In other words, the reduction in total PCBs concentration for the No-Action scenario is about the same as that forecast for the Fifty-Percent Forcing Function scenario. Comparison of the No-Action scenario to the No-Change and the other toxic chemical management forecasts demonstrates that the effectiveness of control action depends upon understanding which forcing functions are controllable and what the future trend in forcing functions will be in the absence of control actions. It could be dangerous to assume that atmospheric vapor concentrations will continue to decline in the future according to the rate of decline observed in the past. Clearly, a better understanding of long-term trends in total PCBs vapor concentrations would lead to more accurate forecasts of toxic chemical concentrations expected from control actions. Ultimately, this will be essential if models are to inform decisions regarding the control of PCBs in Lake Michigan and the other Great Lakes.

2.5.7 Uncertainty of MICHTOX Model Predictions

Model predictions are uncertain for a number of reasons, including: conceptual errors and/or omissions, errors in parameterization, uncharacterized system variability, and systematic errors in forcing functions and calibration data. The uncertainty of MICHTOX predictions, arising from errors in model parameterization and forcing functions, has been evaluated using conventional and BMC analyses. Uncertainty analyses have been conducted on a steady-state version of MICHTOX due to the computational requirements of the methods involved. The results of BMC analysis of the original steady-state model are presented in Table 2.11. The "prior" (*a priori*) results are comparable to conventional Monte Carlo analysis, in which the uncertainty of parameters and forcing functions is defined as uncorrelated probability distributions. The parameters and forcing functions used to generate the posterior results have been "informed" by application of the likelihood function (Dilks *et al*., 1992) based upon the residuals between model predictions and confirmation data. In other words, the reduction in uncertainty evident in the posterior results (indicated by the 95% confidence intervals in Table 2.11) reflects the utility of the confirmation data. Although the BMC analysis shown here was conducted prior to the availability of the LMMBP data, the results are expected to be representative of the uncertainty in MICHTOX total PCBs predictions: total PCBs concentrations should be well within a factor of two of the model predictions. It is also possible that repeating the BMC analysis using LMMBP data and forcing functions would result in even smaller confidence intervals for predictions and, hence, less uncertainty.

2.5.8 Are Lake Michigan Total PCBs Concentrations in Equilibrium With Atmospheric Vapor Concentrations?

For the past decade, scientists have debated whether PCBs concentrations in the Great Lakes

Table 2.11. Results of BMC Uncertainty Analysis for Original Steady-State MICHTOX Model

Model State Variable	Units	Prior Total PCBs Concentration Predictions: Mean	Prior Total PCBs Concentration Predictions: 95% Confidence Interval	Posterior Total PCBs Concentration Predictions: Mean	Posterior Total PCBs Concentration Predictions: 95% Confidence Interval
Water Column	ng/L	0.280	(0.14 - 0.57)	0.297	(0.20 - 0.44)
Surficial Sediments	ng/g	62.6	(30 - 130)	71.4	(48 - 105)
Lake Trout	ng/g	2354	(720 - 7700)	2620	(1700 - 4100)

have reached a state of equilibrium with atmospheric vapor concentrations (International Joint Commission, 1996; Stowe *et al*., 1995; Smith, 1995, 2000; U.S. Environmental Protection Agency, 1993). This interpretation is an alternative to the hypothesis that PCBs concentrations largely reflect the resuspension of PCBs from the lake sediments or other ongoing sources such as tributaries. Obviously, the outcome of this debate has significant implications regarding how best to manage PCBs and possibly other toxic chemicals in Lake Michigan and the other Great Lakes (as was illustrated by the forecasts of toxic chemical management alternatives) and was a primary motivation for conducting the LMMBP.

Figure 2.33 plots the observed trends of total PCBs concentrations in air (vapor concentrations for the Great Lakes region reported by Schneider *et al*., 2001) and Lake Michigan water. The similarity between these trends suggests that PCBs concentrations may be at or near equilibrium. To explore this further, predictions from the No-Action forecast scenario were used to calculate the water-to-vapor ratio of total PCBs concentrations (dissolved total PCBs concentration in water/atmospheric vapor total PCBs concentration). The result, plotted in Figure 2.34, indicates that for this scenario, the water-to-vapor concentration ratio increases with time. Therefore, the model does not predict equilibrium between air and water total PCBs concentrations. This analysis should be repeated for other forcing function scenarios to determine whether this result is general or specific to the forcing function assumption.

2.5.9 Sensitivity of Bioaccumulation Predictions to Initial Total PCBs Concentrations in Fish

Models such as MICHTOX are generally quite sensitive to initial concentration conditions. Total PCBs concentration predictions from the initial years of the forecast scenarios (Figure 2.32) display a transient increase, which is attributable to initial conditions in the model. Tests of the bioaccumulation model sensitivity to initial conditions indicated that the model predictions were not sensitive to initial conditions after a number of years equal to the age class of fish being examined. This is illustrated in Figure 2.35, where substantially different initial total PCBs concentrations were used for the two simulations. Comparison of predictions for age seven lake trout show that sensitivity to initial conditions disappears within the first six to seven years of simulation. Therefore, the five- and ten-year predictions for toxic chemical management forecasts (Figure 2.32 and Table 2.10) do not depend upon the specification of initial total PCBs concentrations in fish.

2.5.10 Sensitivity of Bioaccumulation Predictions to Food Chain Model Parameterization

Confirmation of the total PCBs bioaccumulation predictions for both steady-state exposure (Figures 2.10 and 2.11) and Scenario B simulations (Figures 2.25 and 2.26) suggest that predictions are biased low by 20-30% for most fish age and size classes. Recalibration of the MICHTOX food chain model may

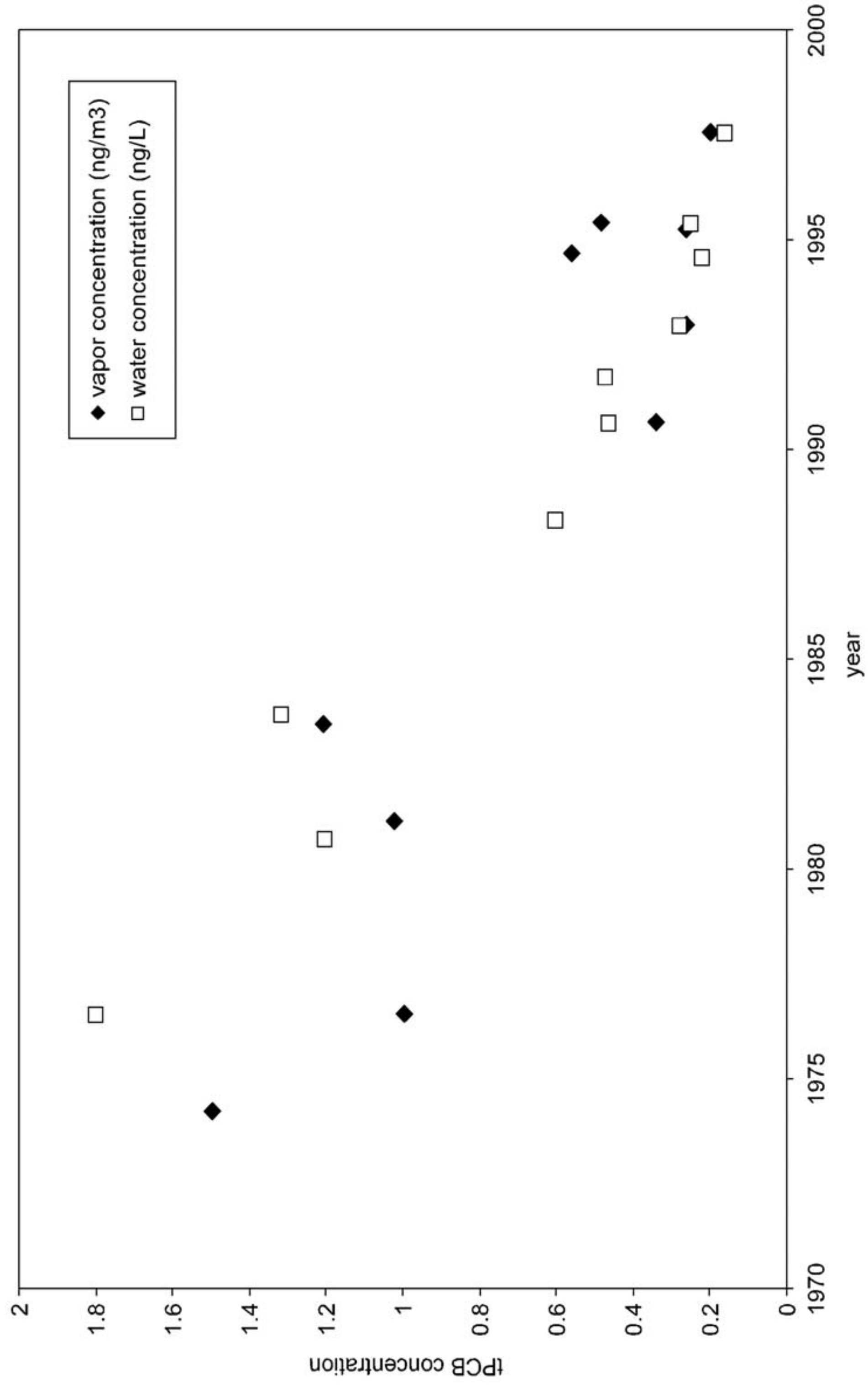

Figure 2.33. Total PCBs concentrations in Lake Michigan air and water.

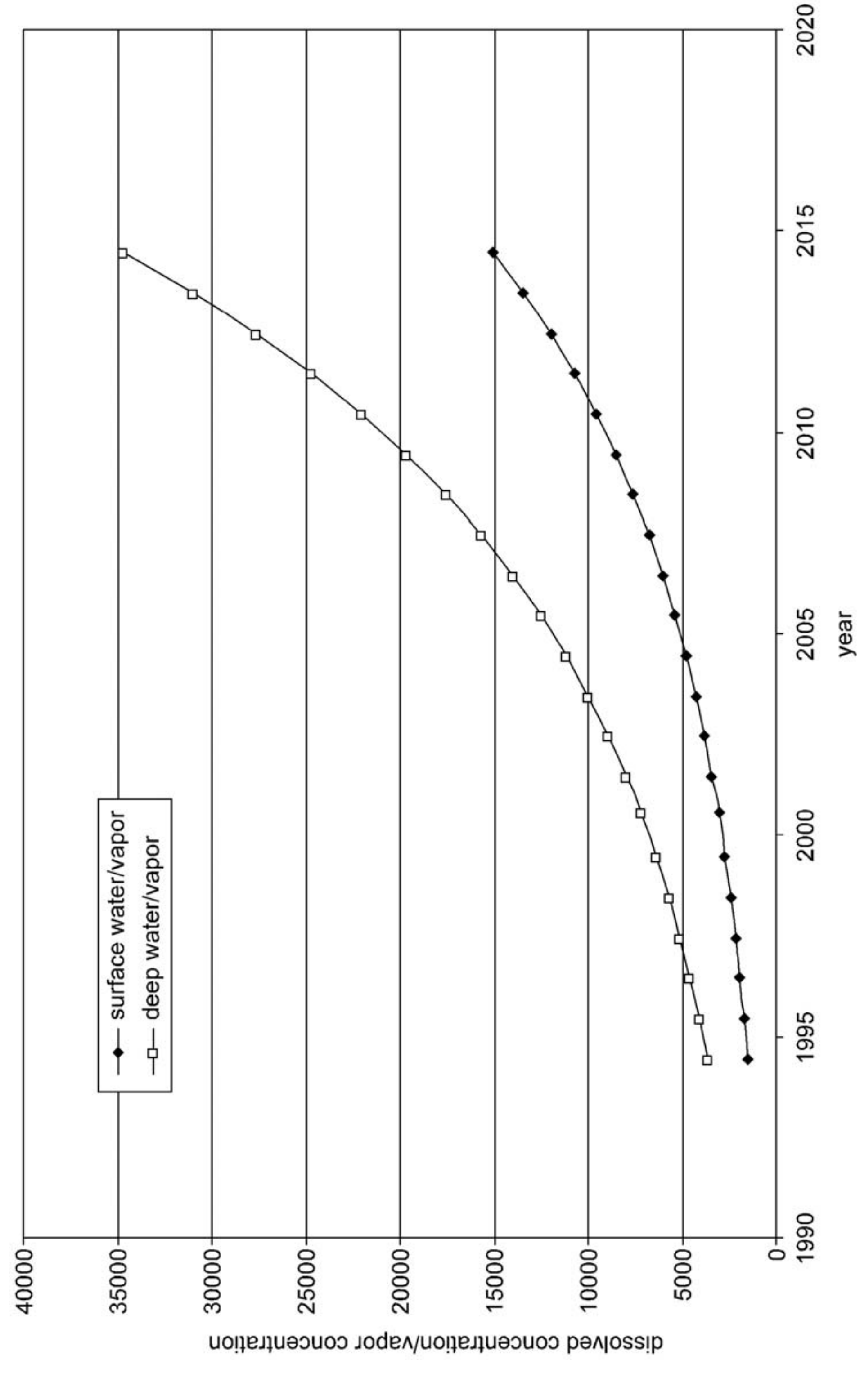

Figure 2.34. Ratio of total PCBs concentrations between dissolved water and vapor (MICHTOX No-Action forecast).

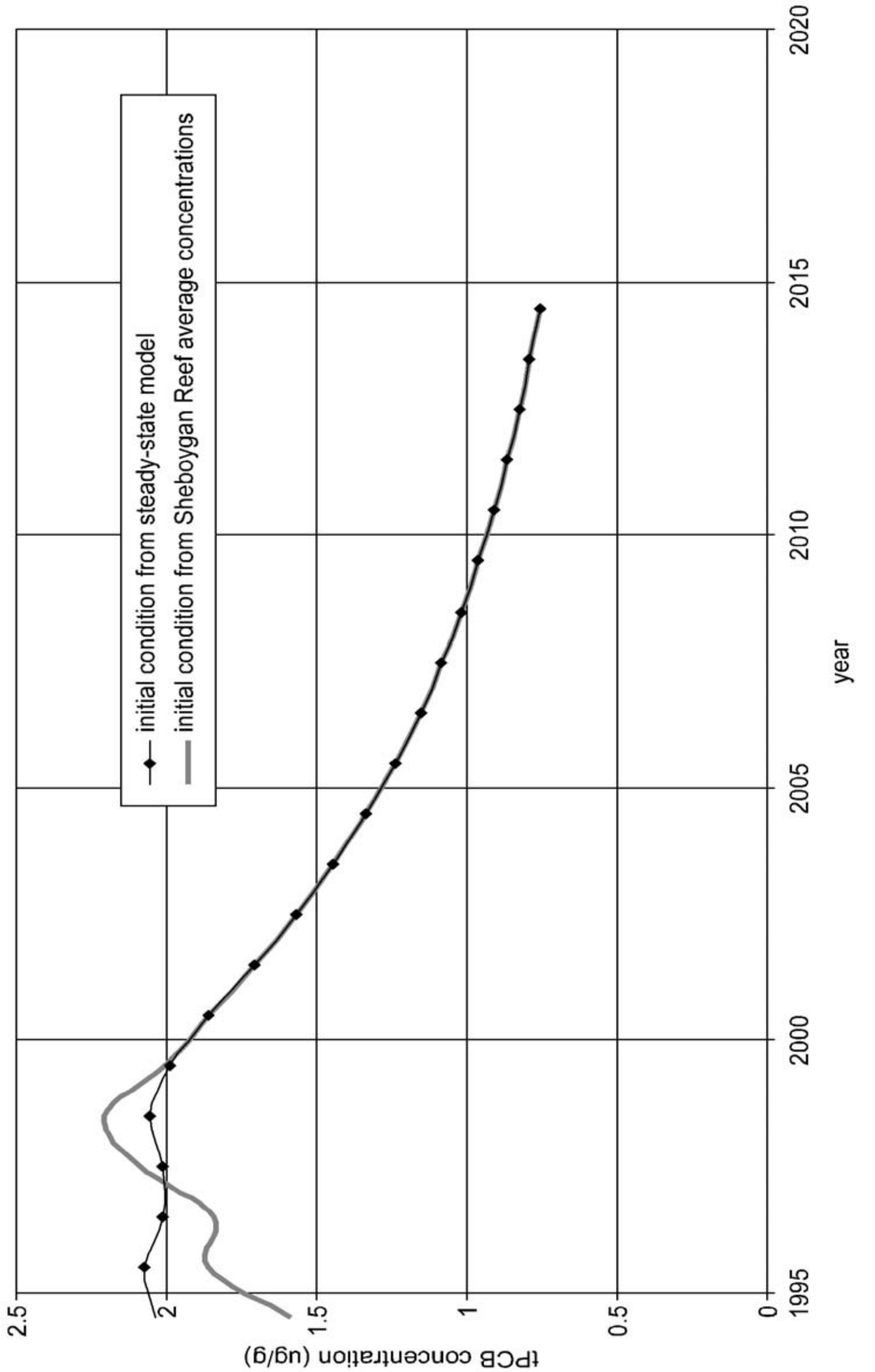

Figure 2.35. Sensitivity of food chain model to initial conditions. Age seven lake trout: No-Change forecast.

be appropriate, given that the parameterization of this model has never been optimized using field data. Although recalibration was beyond the scope of this project, sensitivity analysis was used to demonstrate that an optimal fit of the LMMBP total PCBs data could be readily achieved by adjusting a single food chain model parameter. The parameter of interest, the chemical assimilation efficiency, was increased to 0.8. This was the maximum value suggested by the literature and prior model applications. Comparisons of the model predictions, made with this parameter adjustment, to the initial model predictions and the data for total PCBs concentrations in fish at Saugatuck, are presented in Figure 2.36. Adjustment of chemical assimilation efficiency alone increases the total PCBs concentrations predicted by the food chain model by over 50%. Other important bioaccumulation parameters, including diet composition, growth rates, lipid contents, chemical excretion rates, and phytoplankton bioconcentration factors, should also be examined in any recalibration effort. However, sensitivity analysis demonstrates that it should be possible to optimize the bioaccumulation predictions to data collected in either Saugatuck or Sheboygan Reef biota zones or some aggregation of these data.

2.5.11 Are Total PCBs Bioaccumulation Factors Constant for Lake Trout in Lake Michigan?

Bioaccumulation factors (BAFs) are defined as the ratio of chemical concentration in fish (normalized by fish lipid content) to dissolved concentrations in water. BAFs are often used as simple substitutes for food chain model predictions, for example to estimate chemical concentrations in fish from measured concentrations in water (U.S. Environmental Protection Agency, 2000). However, BAFs are not necessarily constant in the ecosystem. This can be demonstrated by calculating BAFs from the food chain model results. BAFs calculated from the No-Change forecast scenario, plotted in Figure 2.37, show that BAFs vary continuously throughout the simulation. The BAFs initially increase rapidly, reach a maximum of over 7×10^7, and then decline at a constant rate for the duration of the simulation. Thus, BAFs should be used with caution in Lake Michigan, as they are expected to vary with time.

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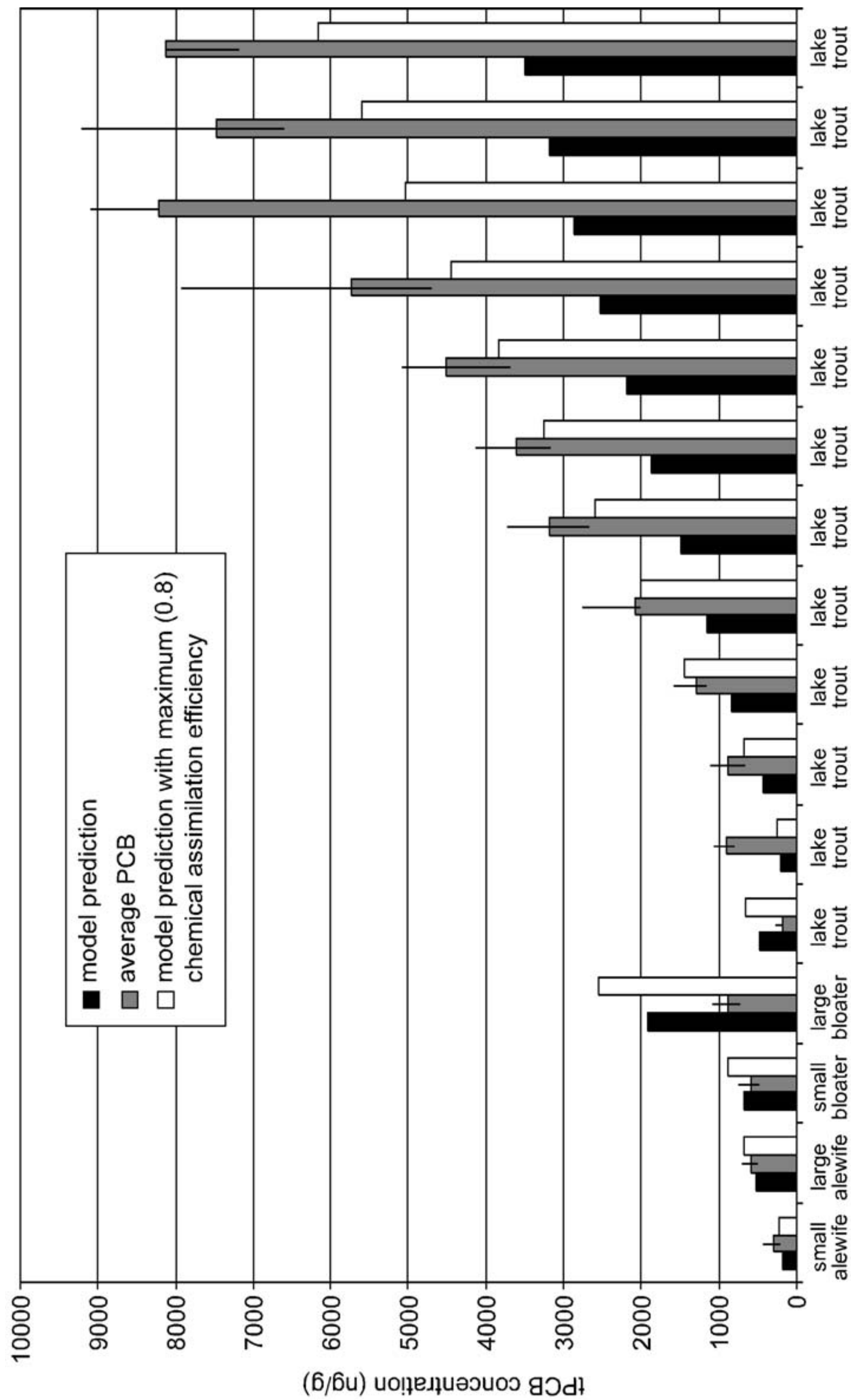

Figure 2.36. Sensitivity of MICHTOX steady-state PCBs concentrations to chemical assimilation efficiency and comparison to Saugatuck biota zone data.

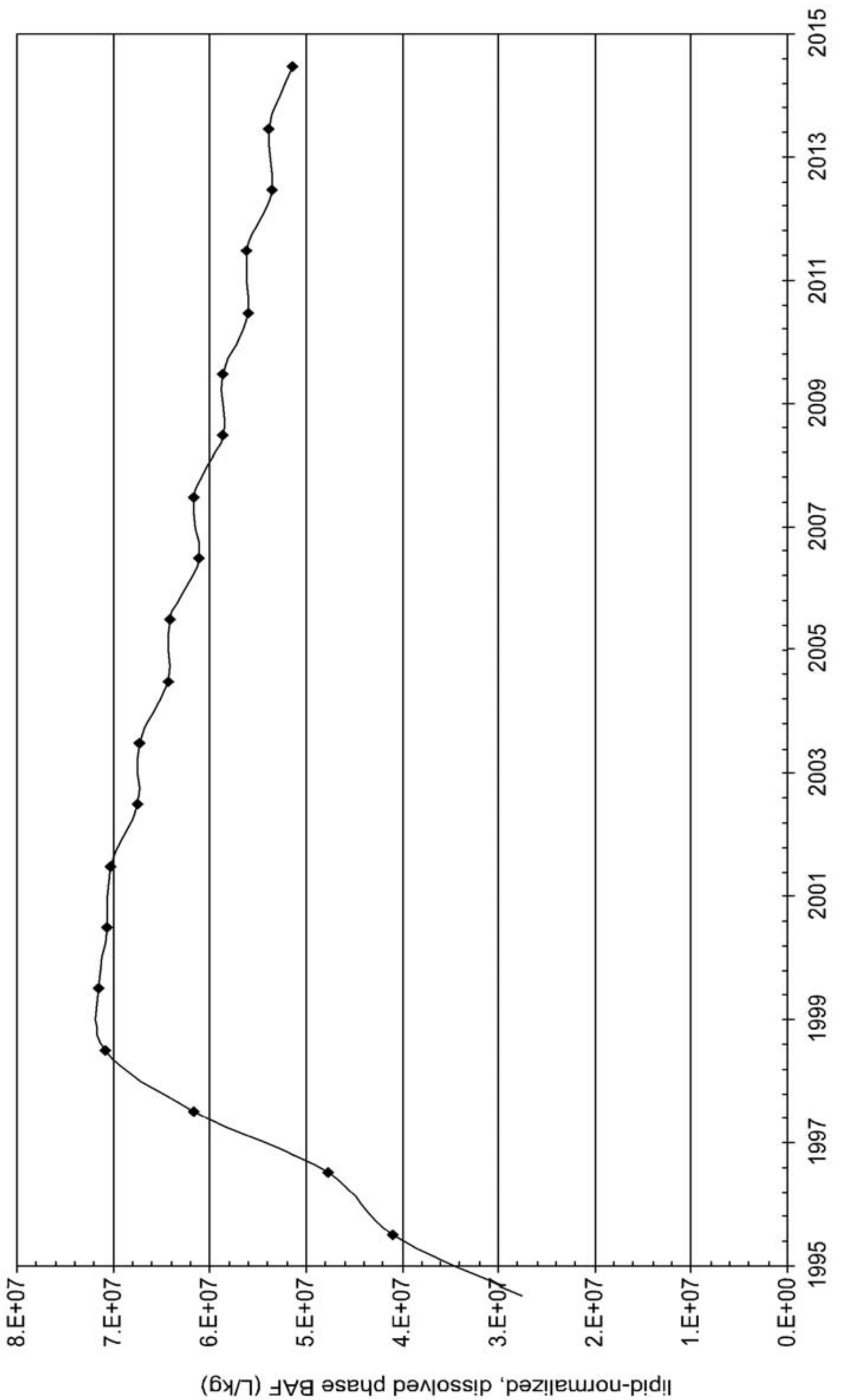

Figure 2.37. Predicted bioaccumulation factors for total PCBs in age seven lake trout (No-Change forecast simulation).

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